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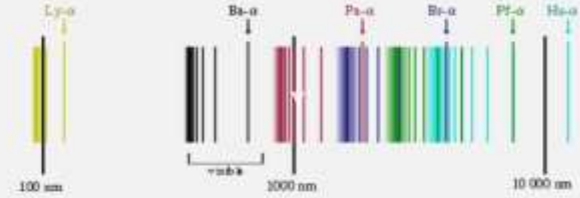
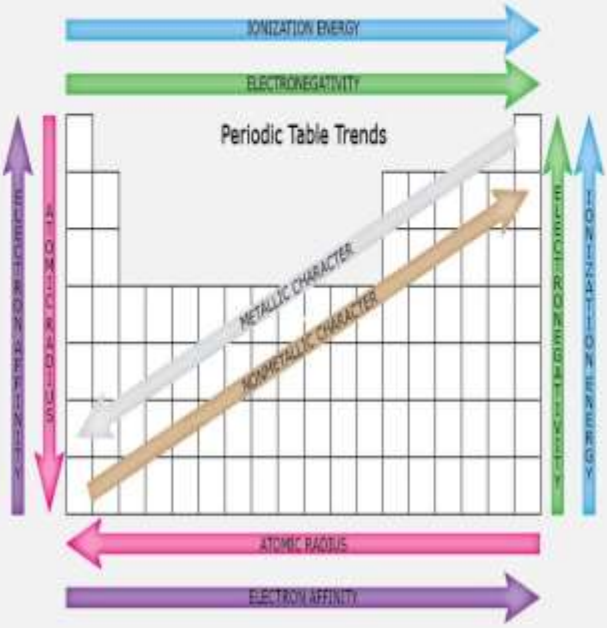


Inorganic Chemistry

First Year lectures



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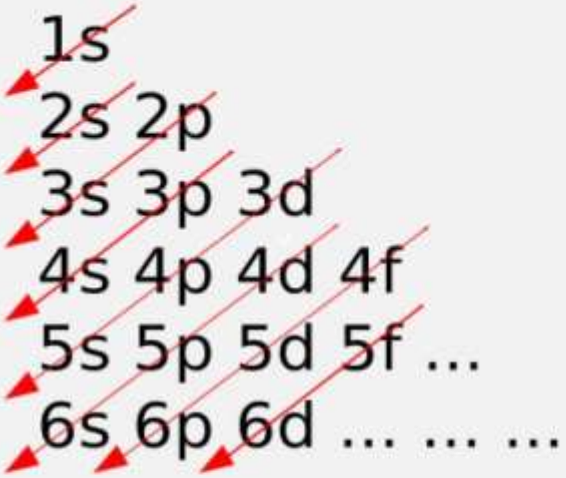


Part -I-

CHAPTER ONE

INORGANIC CHEMISTRY

Chapter One

Inorganic Chemistry

Basic concepts: Atoms

1. Fundamental Particles of an atom

An atom is the smallest unit quantity of an element capable of existence, either alone or in chemical combination with other atoms of the same element or another element. The fundamental particles of an atom are the proton, electron and neutron, proton and neutron have approximately the same mass, relative to these electron has negligible mass the charge on a proton is positive and of equal magnitude, but opposite sign, to that on negatively charged electron, a neutron has no charge. In an atom of any element there are equal number of protons and electrons and so an atom is neutral.

The nucleus of an atom consist of proton and neutrons (with the exception of protium its nucleus consists of single proton). The nucleus is positively charged and the electrons occupy a region of space around the nucleus, nearly all the mass of an atom is concentrated in the nucleus but the volume of the nucleus is only a tiny fraction of that of the atom the radius of the nucleus is about 10^{-5} m while the atom itself is a 10^{5} time larger than this(calculated the radius of an atom in cm?)

2. Atomic number, mass number and isotopes

Atomic number Z=number of protons in the nucleus=number of electrons

Mass number A= number of protons+ number of neutrons

number of neutrons **= A-Z**

mass number → A

E ← **Element**

atomic number → Z

eg : $^{14.0064}_{7}N$ $^{35.45}_{17}\mathbf{Cl}$ $^{65.37}_{30}\mathbf{Zn}$ $^{22.96}_{11}\mathbf{Na}$

3. Unit of atomic mass number

Since the proton mass **=1.672×10^{-24} g**

and the neutron mass **=1.674×10^{-24} g**

So it is convenient to use the atomic mass unit (amu **= 1.66×10^{-24} g**) as a unit for atomic mass number **A**.

Calculate the atomic mass number of carbon atom in terms of **(amu)**.

Carbon nucleus contain **(6)** proton **&(6)** neutrons

A = 6P+6n

$$=\frac{6*1.672*10^{-24}}{1.66*10^{-24}}+\frac{6*1.674*10^{-24}}{1.66*10^{-24}} = 12.0939$$

4. Isotopes

Nuclides of the same element possess the same number of protons and electrons but differ in the number of neutrons so their mass number is differ are called isotopes. The isotopes of some elements occur naturally while other may be produced artificially.

eg: $^{16}_{8}\mathrm{O}$ $^{17}_{8}\mathrm{O}$ $^{18}_{8}\mathrm{O}$

$^{12}_{6}\mathrm{C}$ $^{13}_{6}\mathrm{C}$

$^{1}_{1}\mathrm{H}$ $^{2}_{1}\mathrm{D}$ $^{3}_{1}\mathrm{T}$

Elements that have no isotopes called monotropic **eg**: $^{31}_{15}\mathrm{P}$

Relative atomic mass (Ar)

The relative atomic mass **(Ar)** of the element is the weighted of the mass number of all isotopes.

Ex$_1$: Calculate the value of Ar for naturally occurring chlorine if the distribution of isotopes is **75.77%** $^{35}_{17}\mathrm{Cl}$ and **24.23%** $^{37}_{17}\mathrm{Cl}$ Accurate masses for $^{35}\mathrm{Cl}$ and $^{37}\mathrm{Cl}$ are **34.47 & 36.97** .

$$\mathbf{Ar} = \left(\frac{75.77}{100}*34.47\right)+\left(\frac{24.23}{100}*36.97\right)$$

= 35.45

Ex$_2$: Calculate **Ar** for naturally occurring **Mg** if the isotopes distribution is **78.99%** **^{24}Mg, 10.00%** **^{25}Mg** and **11.01%** **^{26}Mg** Accurate masses are **23.99, 24.99, & 25.98**

$$\mathbf{Ar} = \left(\frac{78.99}{100} * 23.99\right) + \left(\frac{10}{100} * 24.99\right) + \left(\frac{11.01}{100} \times 25.98\right)$$

$$= 24.306$$

Quantum theory:

In **1901,** Plank suggested that energy could be absorbed or emitted only in quanta of magnitude **ΔE** related to the frequency of radiation ς by equation **(1)**

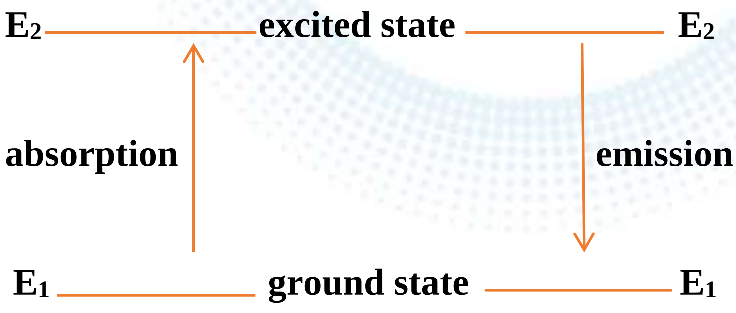
$\Delta E = h\upsilon$…….(1) units: E in J, υ in s^{-1} or Hz

$c = \lambda\upsilon$………(2) units: λ in m, υ in s^{-1} or Hz

$\therefore \Delta E = h\frac{c}{\lambda}$**…..(3) c** = the speed of light in a vacuum = **2.99×10^{8} ms^{-1}**

When energy is provided (as heat or light) to an atom or other species, one or more electron may be promoted from a ground state level to a higher energy state

This excited state is transient and the electron falls back to the ground state, this produce an emission spectrum.



$\Delta E = E_2 - E_1$……….(4)

The emission spectrum of atomic hydrogen

One of the most important applications of early quantum theory was the interpretation of atomic spectrum of hydrogen on the bases of Rutherford-Bohr model of the atom.

When an electric discharge is passed through a sample of dihydrogen the $\mathbf{H_2}$ molecules dissociate into atoms and the electron in particular excited **H** atom may be promoted to one of many high energy levels. These states are transient and the electron falls down to a lower energy state, emitting energy as dose so. The consequence is the observation of spectral lines in the emission spectrum of hydrogen the spectrum **(Fig.1)** consists of groups of discrete lines corresponding to electronic transitions each of discrete energy. All lines in all series obey the general expression given in equation **(5)**

$$\bar{\boldsymbol{\upsilon}} = \frac{\mathbf{1}}{\boldsymbol{\lambda}} = \boldsymbol{R}\left(\frac{\mathbf{1}}{\boldsymbol{n}^2} - \frac{\mathbf{1}}{{}'\boldsymbol{n}^2}\right)\text{…………..}\mathbf{(5)}$$

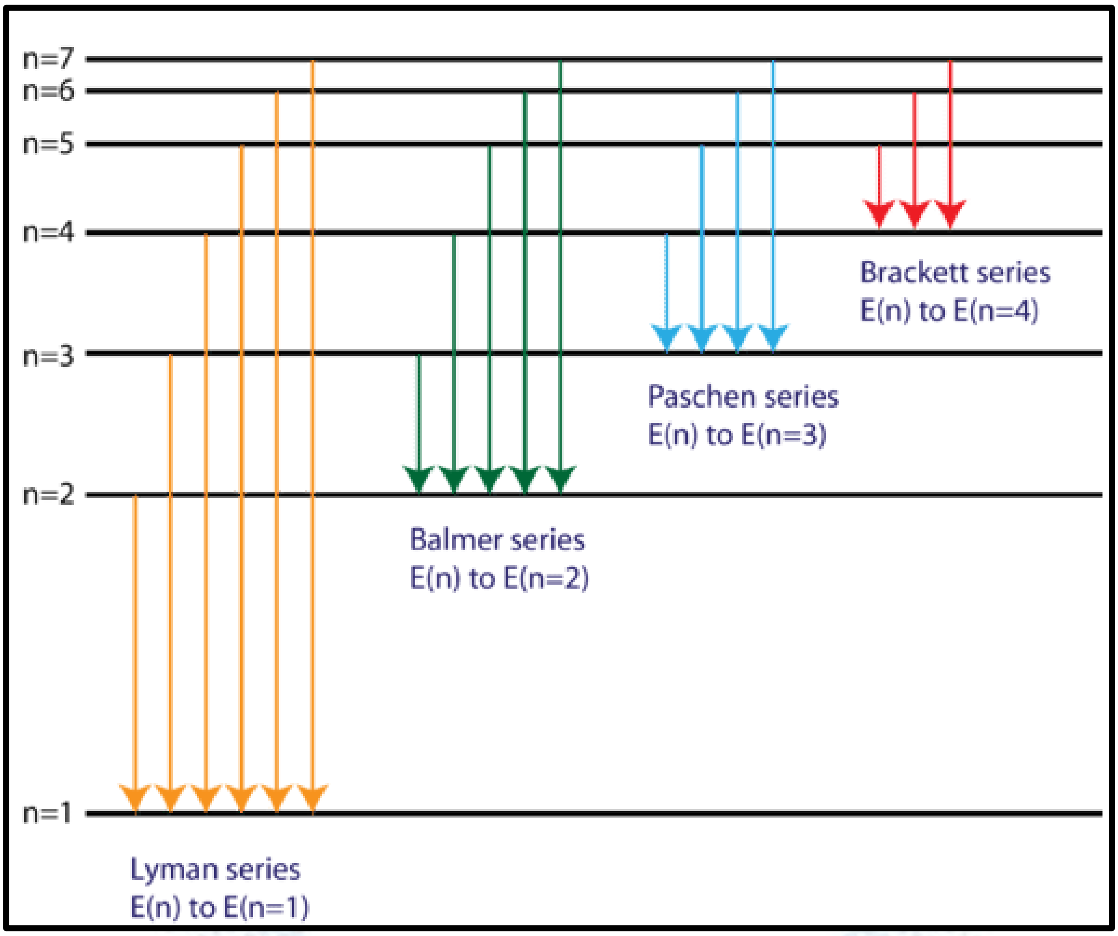
Where $\mathbf{n}' > \mathbf{n}$ **R** = Rydberg constant for
Hydrogen = $\mathbf{1.097 \times 10^{7} m^{-1}}$
$\mathbf{= 1.097 \times 10^{5} cm^{-1}}$

For Lyman series **n =1**

For Balmer series **n =2**

And for Paschen, Brakett and Pfund series
n = 3, **4** and **5** respectively

Fig: (1) The emission spectrum of atomic hydrogen electron transitions for thy Hydrogen atom



Ex: state which of the following **n′→n** transition in the emission spectrum of atomic hydrogen belong the Balmer, Lyman or Paschen series **(a) 3→1; (b) 3→2 ; (c) 4→3 ; (d) 4→2 ; (e) 5→1**

Bohr's theory

In **1913** Nils Bohr combined elements of quantum theory and classical physics in a treatment of hydrogen atom. **He** states two postulates for an electron in an atom:

1. Stationary states exist in which the energy of the electron is constant, such states are characterized by circular orbit about the nucleus in which the electron has an angular momentum **(Mvr)** given by eqn. **(6)**

$$\mathbf{Mvr = n\left(\frac{h}{2\pi}\right) \ldots\ldots\ldots\ldots (6)}$$

n = the principle quantum number

m = mass of electron; **v =** velocity of electron

r = radius of the orbit ; **h=** Plank constant $^{n}/_{2\pi}$ may be written as **ħ**

2. Energy is absorbed or emitted when an electron moves from one stationary state to another and the energy change is given by equation**(7)**

$\Delta\mathbf{E} = \mathbf{E}\boldsymbol{n_2} - \mathbf{E}\boldsymbol{n_1}$**……….(7)**

Bohr model for hydrogen atom

If Bohr's model is applied to the hydrogen atom the radius of **H**-atom **&** it ionization energy could be obtained by using the following equation **(8&9)**

$\boldsymbol{r_n \propto n^2}$

$\boldsymbol{r_n = a_0 n^2}$**…………..(8)**

r = the orbit radius

n = principle quantum number

a_0 = constant=**0.53A^0**

for H-atom **n = 1**

$\boldsymbol{r_1 = a_0 * 1^2 = a_0 = 0.53A}$ this value is called the Bohr radius of **H**-atom

Ex: calculate the radii of the **2nd ,3rd& 4th** orbit of the **H**-atom, what do you conclude ?

$\boldsymbol{r_n = \ a_0 n^2}$

$\boldsymbol{r_2 = a_0 2^2 = 0.53 * 4 = }$ **2.12 A^0**

$\boldsymbol{r_3 = a_2 3^2 = 0.53 * 9 = }$ **4.77 A^0**

$\boldsymbol{r_4 = a_0 4^2 = 0.53 * 16 = }$ **8.48 A^0**

An increase in the principle quantum number from **n=1 to n=**∞ has special significance. It corresponds to the ionization of the atom **(equation 9)** and the ionization energy **(IE)**, can be determined by combining **eqs 5 &7** as shown in equation **………. (9)**

$\mathbf{H}_{(g)} \rightarrow \mathbf{H}^{+}_{(g)} + \bar{e}$

n = 1 **n = ∞**

$\mathbf{IE} = \mathbf{E}_{\infty} - \mathbf{E}_{1} = \frac{hc}{\lambda} = hcR\left(\frac{1}{1^2} - \frac{1}{\infty^2}\right)$**……….(9)**

h = Plank constant = $\mathbf{6.62\times10^{-34}Js}$

c = velocity of light = $\mathbf{3\times10^{10}cms^{-1}}$

R= Rydberg constant = $\mathbf{1.097\times10^{5}cm^{-1}}$

IE = hcR**(1-0)**

= $\mathbf{2.179\times10^{-18}J}$

For ℓ mole of hydrogen, Avogadro number = $\mathbf{6.022\times10^{23}\ mol^{-1}}$

IE = $\mathbf{2.179\times10^{-18}\times6.022\times10^{23} = 1.321\times10^{6}J\ mol^{-1}}$

$\mathbf{=1312KJ\ mol^{-1}}$

Ionization energy is often expressed in electron volts **(eV)**

1 ev = 96.4853≈96.5 KJ $\mathbf{mol^{-1}}$

∴ I.E of H can be also given as **13.60 eV**

The wave nature of electron:

In **1924** Louis de Broglie argued that if light were composed of particals (As Albert Einsetin implies a partical theory of light and the quantum theory of radiation introduced by Max Plank) and yet showed wave like properties, the same should be true of electrons and other particals. This phenomenon is refered as wave-partical duality.

$\mathbf{E = h\upsilon}$ Max Plank

$\mathbf{E = mc^2}$ Enisetin

$\mathbf{h\upsilon = mc^2}$

$\mathbf{h\frac{c}{\lambda} = mc^2}$

$\mathbf{\frac{h}{\lambda} = mc = p} \quad \therefore \quad \boldsymbol{\lambda} = \mathbf{\frac{h}{p} = \frac{h}{mv}}$

The uncertainty principle:

It is impossible to know the exact position **(x)** and the same momentum **(m.v)** of partical at the same instant of time

$$\Delta \mathbf{x}\ \mathbf{m}\Delta \mathbf{v} \geq \frac{\mathbf{h}}{\mathbf{4\pi}}$$

$\Delta \mathbf{x}$ the uncertainty in position

$\Delta \mathbf{v}$ the uncertainty in speed

Probability of finding the electron in a given volume of space which is given by the function $\boldsymbol{\psi}^2$where $\boldsymbol{\psi}$ is the mathematical symbol called the wave function which describes the behaviour of an electron wave.

The wave function $\boldsymbol{\psi}$ is the solution of schrodinger equation which describe the behaviour of an electron wave a region of space called atomic orbital.

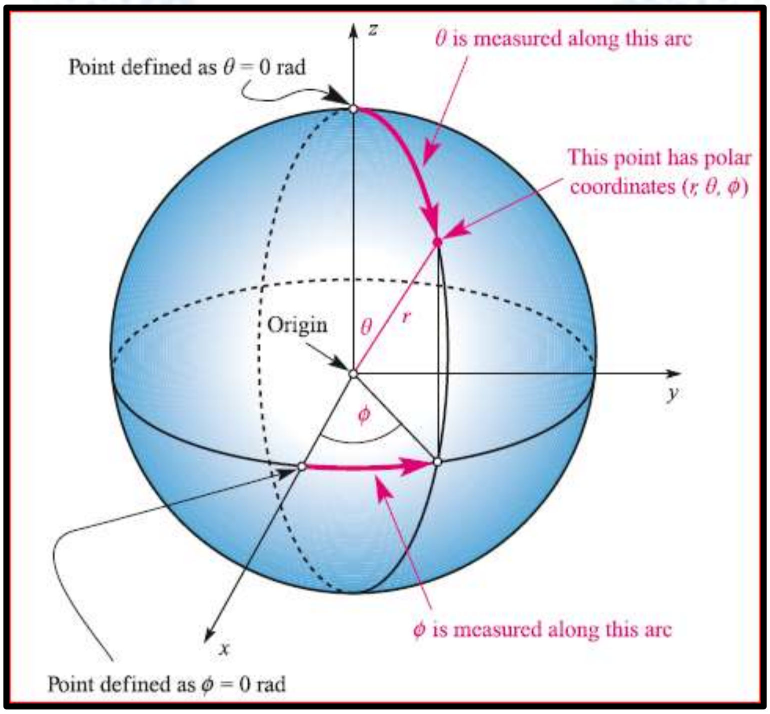
The wave function $\boldsymbol{\psi}$ is consist of radial component $\mathbf{R}_{(\mathbf{r})}$ and an angular component $\mathbf{A}(\boldsymbol{\theta}, \emptyset)$

[see Fig-2-]

$$\boldsymbol{\psi}_{\mathbf{cartesian}_{(X,Y,Z)}} = \boldsymbol{\psi}_{\mathbf{radial}(\mathbf{r})}\boldsymbol{\psi}_{\mathbf{angular}}(\boldsymbol{\theta}, \emptyset)$$

$$= \mathbf{R}_{(\mathbf{r})}\mathbf{A}(\boldsymbol{\theta}, \emptyset)$$

Fig. (2): Defintion of polar coordinates (r, Ө, φ) and cartesian coordinates (x, y, z) also shown.



Atomic Orbital

An atomic orbital is usually described in terms of three integeral quantum numbers

1. The principle quantum number n which is a positive integer it values lying between the limits $\mathbf{1 \le n \le \infty}$ allowed values of n arise when the radial part of wave function is solved the value of n determine the size of orbital **&** its radius.

2. Orbital quantum number $(\boldsymbol{\ell})$ has allowed values $\mathbf{0, 1, 2, \ldots .}\,(\boldsymbol{n-1})$. The value of $\boldsymbol{\ell}$ determine:

- **a.** The shape of the atomic orbital
- **b.** The orbital angular momentum

$$= \left[\sqrt{\boldsymbol{\ell(\ell+1)}}\right]\frac{\boldsymbol{h}}{\boldsymbol{2\pi}}$$

It appers when the angular part of wave function $\boldsymbol{\psi_{\theta,\emptyset}}$ is solved.

According to **(ℓ)** values four types of atomic orbitals arise **ℓ**, which are different in shapes and symmetry such orbital are:

s p d f

ℓ = 0 1 2 3

each atomic orbital is associated with principle quantum number **(n)** like

1s 2s 2p 3s 3p 3d 4s 4p 4d 4f

n = 1 2 3 4

3. Magnetic quantum number **ml** its value gives information about the directionalty of an atomic orbital and has integral values between +l…..-l

number of **(m_ℓ)** value **= 2ℓ+1**

(m_ℓ) appers when the radial part of wave function $\boldsymbol{\psi_{\theta\emptyset}}$ is solved

Ex: 1. Given that the principle quantum number is **2** write down the allowed values of **ℓ & m_ℓ**, and determine the number of atomic orbitals possible for **n = 3**

when **n = 2** $\therefore \ell = 0, 1$

$m_\ell = 0, +1, 0, -1$

n = 3 $\ell = 0,1,2$

$m_\ell = 0, +1, 0, -1 , +2, +1, 0, -1, -2$

2. If m_ℓ has values of **+1, 0, -1**, write down the corresponding value of ℓ

$m_\ell = +1,0,-1 \quad \therefore \ell=1$

3. If ℓ has values of **0,1,2 &3** deduce the corresponding value of **n**

4. If **n = 1** what are the allowed values of ℓ **&** m_ℓ

n=1 $\ell=0 \quad m_\ell=0$

5. Complete the following sets of quantum numbers

a. **n=4** $\ell=0,1,2,3$

$m_\ell = 0,+1,0,-1;+2,+1,0,-1,-2;+3,+2,+1,0,-1,-2,-3$

b. **n=3** $\ell=0,1,2$

$m\,\ell= 0, (+1, 0, -1), (+2, +1, 0, -1, -2)$

6. Using the rules that govern the values of the quantum numbers **n &** ℓ write down the possible types of atomic orbitals for **n=1,2 , 3 and 4.**

for **n=1** $\ell=0$ ∴**1s** orbital

n=2 $\ell=0,1$ ∴**2s & 2p** orbitals

n=3 $\ell=0,1,2$ ∴**3s 3p & 3d** orbitals

n=4 $\ell= 0, 1, 2, 3$ ∴ **4s 4p 4d 4f orbitals**

7. Which atomic orbital has values of **n=4 &** $\ell=2$

n=4 $\ell=0,1,2,$ ∴**4d** orbital

8. Give the three quantum numbers that describe **2s** atomic orbital

n=2 $\ell=0 \quad m_\ell=0$

9. Which quantum number that distinguishes the

3s and **5s** atomic orbitals

the **3s** & **3d** atomic orbitals

the five **3d** atomic orbitals

the three **p** atomic orbitals

The physical discrption of atomic orbitals

The accepted solution of schrodinger equation give a physical discrption for the atomic orbital as a region of space at which the probability (ψ^2)of finding electron is very high **(>95%)**.

1. For s-orbital such solution is independent on $\boldsymbol{\theta}$ & $\emptyset$ ($\mathbf{A}_{\theta,\emptyset}$) but it depends only on $\mathbf{R}_{(r)}$, so s-orbital is spherically symmetrical

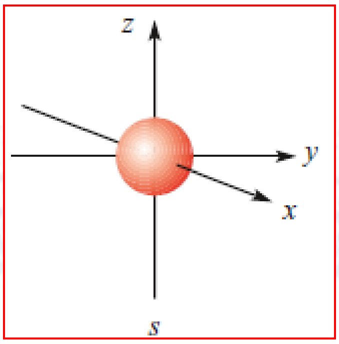


Fig 3: s-orbital

For s-orbital $\boldsymbol{\ell=0}$ so s-orbital is singly degenerate

2. The p-orbital is 3- fold degenerate or triply degenerate (degenerate orbitals possess the same energy)

The schrodinger solutions for p-orbitals depends on both $\mathbf{R}_{(r)}$ **&** ($\mathbf{A}_{\theta,\emptyset}$) therefore p- orbitals are not spherically symmetrical. It consist of two lopes (dumb-bell) shaped as shown below Fig4:

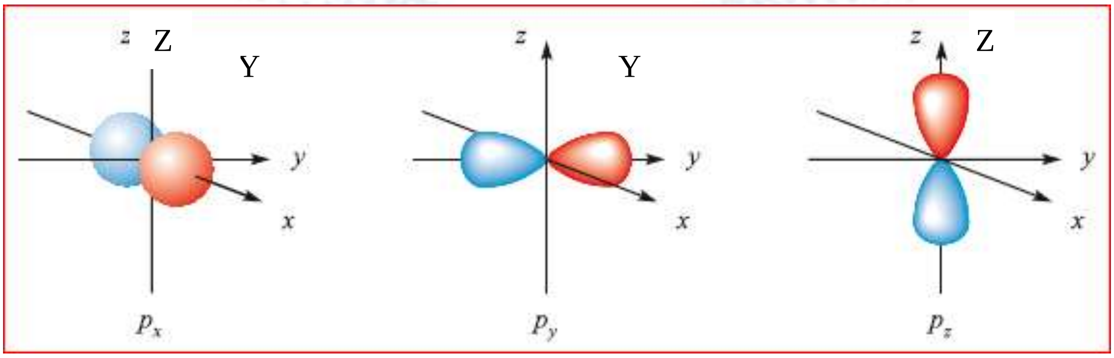


Fig 4:p-orbitals
(+ & -) sign of the wave function

3. For **d-** orbital **$\ell=2$ $m_\ell= +2,+1,0,-1,-2$** therefore d-orbital is five-fold degenerate and the wave function depends on both **$R_{(r)}$ & $(A_{\theta,\emptyset})$.**

The solutions of schrodinger equation indicate that d-orbital is double-dumb-bell as shown below Fig (5).

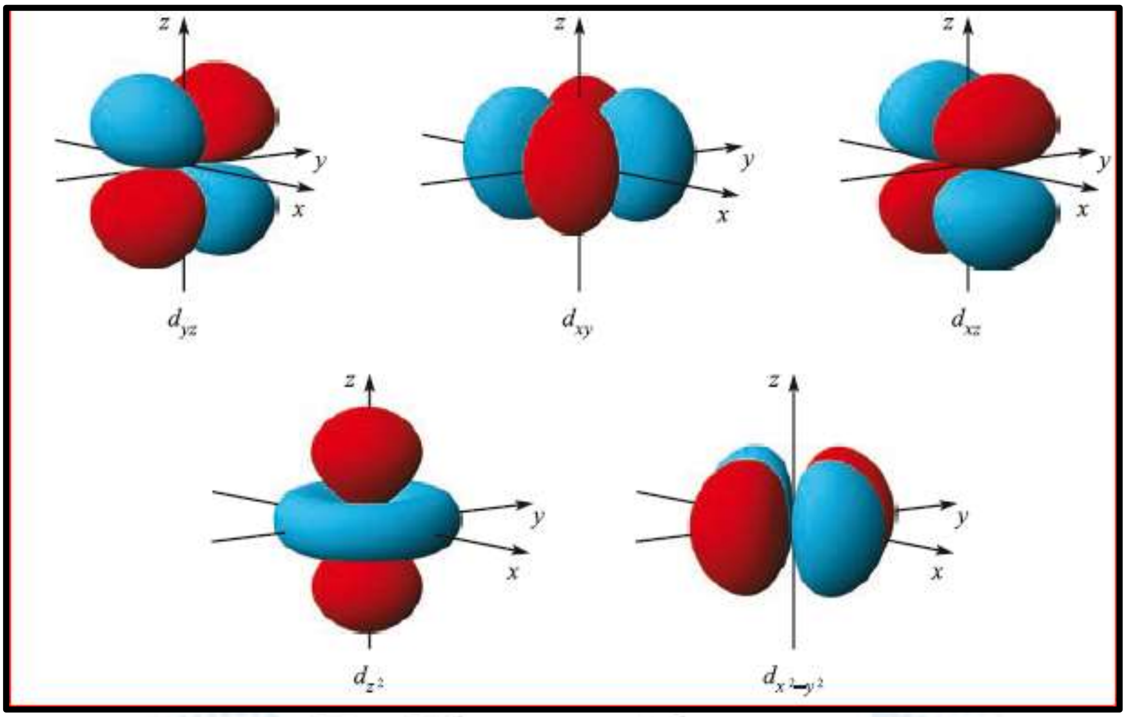


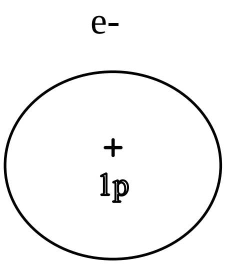
Fig5: d-orbitals

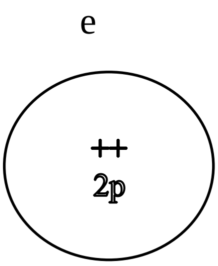
gerad **(g)** and ungerad **(u)** orbitals

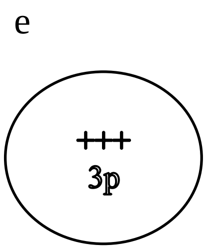
s-and d-orbitals are gerad since the sign at the ends of the line are identical, while p-and f-orbitals are ungerad, the sign at the ends of the line are different.

Orbital energies in hydrogen like species:

Hydrogen like species are atoms, ions, molecules that consists a positive nucleus and one electron **eg: $_2He^+$, $_3Li^{+2}$**







$^{1}_{1}\mathbf{H}$ $\quad$ $\mathbf{{}_2He\ -e \longrightarrow {}_2He^{+}}$ $\quad$ $\mathbf{{}_3Li\ -2e \longrightarrow {}_3Li^{++}}$

$\mathbf{1s^1}$ $\quad$ $\mathbf{1s^2}$ $\quad$ $\mathbf{1s^1}$ $\quad$ $\mathbf{1s^2 2s^1}$ $\quad$ $\mathbf{1s^1}$

1p **1e** $\quad$ **2p** **1e** $\quad$ **3p** **1e**

For such species the solutions of schrondinger eqn. give orbital engergies **E** (energy levels)

$$\mathbf{E = -K\frac{Z^2}{n^2}} \text{ ………….(10)}$$

K=a constant **1.312×10^{3} KJ mol^{-1}**

K=hcR

h=plank's constant **6.62×10^{-34}J.sec**

c=speed of light=**3×10^{10}cms^{-1}**

R=Rydberg constant=**1.097×10^{5}cm^{-1}**

- For each value of n there is only one energy solution
- For hydrogen like species all atomic orbitals with the same **(n) eg : 3s 3p** 3d are degenerate
- The orbital energy levels get closer together as the value of n increase. This result is a general one for other atoms.

Exercieses:

1. Show that the energy of both **2s** and **2p** orbitals for a hydrogen atom is-**328 KJ mol^{-1}**
2. For a hydrogen atom, confirm that the energy of the **3s** orbital is-**1.51eV. (Note: 1eV=96.5KJ mol^{-1})**

4. The spin quantum number

An electron is consider to spin about an axes passing through it and to have spin angular momentum in addition to orbital angular momentum. The spin quantum number determines the magnitude of the spin angular momentum of an electron and has value of $\frac{1}{2}$. Since angular momentum is a vector quantity it must have a direction and this determined by the magnetic spin quantum number **(m_s)** which has a value of $+\frac{1}{2}$ or $-\frac{1}{2}$. Whereas an atomic orbital is defined by a unique set of three quantum numbers, an electron is defined by a unique set of four quantum numbers: **n, ℓ, m_ℓ, m_s.**

As there are only two values of **m_s** an orbital can accommodate only two electrons. An orbital is fully occupied when it contains two spin-paired electrons one electron has **m_s**$=+\frac{1}{2}$ and other has **m_s**$=-\frac{1}{2}$

Ex1: Write down two possible sets of quantum numbers to describe an electron in atomic orbital 3s

$n=3 \quad \ell=0 \quad m_\ell=0 \quad m_s=+\frac{1}{2}$

$n=3 \quad \ell=0 \quad m_\ell=0 \quad m_s=-\frac{1}{2}$

Ex2: If an electron has the quantum numbers

$n=2 \quad \ell=1 \quad m_\ell=-1 \quad m_s=+\frac{1}{2}$ which

type of atomic orbital it occupying

$2p^3$

+1	0	-1
1	1	1

Ex3: write down a set of quantum numbers that describes an electron in 5_s atomic orbital. How does this set of quantum number differ if you are describing the second electron in the same orbital.

For **1st (e)** **n=5** **ℓ=0** **mℓ =0** $m_s=+\frac{1}{2}$

For **2nd(e)** **n=5** **ℓ=0** **mℓ =0** $m_s=-\frac{1}{2}$

The ground state of the hydrogen atom:

The ground state is the most energetically favourable stable.

For H-atom its ground state in which the single electron occupies 1s (lowest-energy) atomic orbital. The electron can be promoted to higher energy orbitals to give excited state.

Energy levels sequence

The following sequence is approximately true in neutral atoms

$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s$

$< 4d < 5p < 6s < 4f < 5d < 6p < 7s < 6d \approx 5f < 7p$

This sequence follows **(n+ℓ)** rule which states that:

1. The orbitals energy increase as **(n+ℓ)** value increase
2. If **(n+ℓ)** value is equal for two or more orbitals, the orbital of the lower energy is that which has lower value of n.

Ex: Rank the following atomic orbitals according to their energy using **(n+ℓ)** rule:

3s 3p

↓ ↓

(n+ℓ)=(3+0) (3+1)

3 4 ∴ **3s < 3p**

4d , 5p , 6s

↓ ↓ ↓

n + ℓ = 4 + 2 , 5 + 1, 6 + 0

=6 , 6 ,6

∴ **4d < 5p < 6s**

The ground state electronic configuration of many electron atoms

This follow aufbau principle in accord with Hund's rule and Pauli exclution principle

1. Orbitals are filled inorder of energy, the lowest energy orbitals being filled first

2.Hund's rule: In a set of degenerate orbitals, electron singly occupied orbitals

3.Pauli exclution principle: No two electrons in an atom have the same set of n, ℓ, mℓ and m_s quantum number.

***** Each orbital can accomodate a maximum of two electrons with different m_s value different spin paired

Ex:

1. write down the ground state configurations for **$_{3}$Li, $_{11}$Na, $_{19}$K& $_{37}$Rb** and comment on the result.
2. How are the ground state electronic configurations of **$_{8}$O, $_{10}$S, $_{34}$Se** alike? Give another element related in the same way.
3. state two elements that have ground state electronic configurations of the general type **[x] ns^{2} np^{1}**, where **x** is a noble gas.

Valance and core electrons

With the exception of H, He and noble gases

The electronic configuration of an element consists of the core electron (noble gas) and the valance electrons that determine the position of the elements in a periodic table as well as its chemistry.

electronic configurations that consists (noble gas core) + valance electrons called: the condensed electronic configuration while: the full electronic configuration is that begining from 1s orbital → **&** so on.

Ex: write the full and the condensed electronic configuration for the following elements: **$_{12}\mathrm{Mg}$, $_{7}\mathrm{N}$, $_{15}\mathrm{P}$, $_{20}\mathrm{Ca}$, $_{26}\mathrm{Fe}$**

$_{12}\mathrm{Mg}$	**$1s^2\ 2s^2\ 2p^6\ 3s^2$**	**$[\mathrm{Ne}]\ 3s^2$**
$_{7}\mathrm{N}$	**$1s^2\ 2s^2\ 2p^3$**	**$[\mathrm{He}]\ 2s^2\ 2p^3$**
$_{15}\mathrm{P}$	**$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^3$**	**$[\mathrm{Ne}]\ 3s^2\ 3p^3$**
$_{20}\mathrm{Ca}$	**$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2$**	**$[\mathrm{Ar}]\ 4s^2$**
$_{26}\mathrm{Fe}$	**$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^6$**	**$[\mathrm{Ar}]\ 4s^2\ 3d^6$**

Periodic table:

The elements in a periodic table is arranged in seven series or periods according to their principle quantum number

1. The first period **n = 1, $_{1}\mathrm{H} \rightarrow {}_{2}\mathrm{He}$** (**2** element)
2. The second period **n=2, $_{3}\mathrm{Li} \rightarrow {}_{10}\mathrm{Ne}$** (**8** element)
3. The third period **n=3, $_{11}\mathrm{Na} \rightarrow {}_{18}\mathrm{Ar}$** (**8** element)
4. The fourth period **n=4, $_{19}\mathrm{K} \rightarrow {}_{36}\mathrm{Kr}$** (**18** element)
5. The fifth period **n=5, $_{37}\mathrm{Rb} \rightarrow {}_{54}\mathrm{Xe}$** (**18** element)
6. The sixth period **n=6, $_{55}\mathrm{Cs} \rightarrow {}_{86}\mathrm{Rn}$** (**32** element)
7. The seventh period **n=7, $_{87}\mathrm{Fr} \rightarrow {}_{118}\mathrm{Og}$** (**32** element)

The elements in a periodic table also arranged groups according to the number of their valance electrons as well as the type of the valance orbitals. There are eight main groups called the representative elements which are:

1. Group**1** elements or the alkali metals of valance shell **ns^1 ($_{3}\mathrm{Li} \rightarrow {}_{87}\mathrm{Fr}$)**
2. Group **2** elements the alkaline earth metals of valance shell **ns^2($_{4}\mathrm{Be} \rightarrow {}_{88}\mathrm{Ra}$)**

(group **1&2**) belong to s-block , while elements from group **13-18** are called p- block elements.

3. Group **13** elements of valance shell **$ns^2\ np^1$ ($_{5}\mathrm{B} \rightarrow {}_{81}\mathrm{Tl}$)**
4. Group **14** elements of valance shell **$ns^2\ np^2$ ($_{6}\mathrm{C} \rightarrow {}_{82}\mathrm{Pb}$)**
5. Group **15** elements called pnictogens of valance shell **$ns^2\ np^3$ ($_{7}\mathrm{N} \rightarrow {}_{83}\mathrm{Bi}$)**
6. Group **16** elements called chalcogenc of valance shell **$ns^2\ np^4$($_{8}\mathrm{O} \rightarrow {}_{84}\mathrm{Po}$)**
7. Group **17** elements called halogens of valance shell **$ns^2\ np^5$($_{9}\mathrm{F} \rightarrow {}_{85}\mathrm{At}$)**
8. Group **18** elements called noble gases of valance shell **$ns^2\ np^6$.($_{2}\mathrm{He} \rightarrow {}_{86}\mathrm{Rn}$)**

The transition metals: they occurred in periods (4-7) and they are two types:

1. Transition metals consist of four series and ten groups **(3-12)** each group consist of **4-**elements, the outer shell electronic configuration is **(ns(n-1) d with n≥4)** they called d-block element
2. The inner transition metals consist of two series the lanthanids and the actindes each series is consist of **14** elements and all occurred in a **14** groups **(3F-16F)** each group consist of two elements. The outer shell electronic configuration is **(ns (n-2) f, n ≥ 6)**, they called f-block element.

Spin- orbital coupling

There is an overlape between the orbital angular momentum of an electron and its spin angular momentum such overlape is described by another quantum number J.

How to find J

1. **j-j** coupling this method is used with elements of atomic number **Z≥30**, here the j value of each electron is calculated **(i.e: ℓ & s of** each electron is taken alone) and the resultant is found:

   $\mathbf{J = \sum j}$ each $\mathbf{j = m_l + m_s}$
2. Resull **-** Saunder's coupling
3. also called spin orbital coupling **(L+S)**

   $\mathbf{L = \sum(m_\ell)}$ for all electrons

   $\mathbf{S = \sum(m_s)}$ for all electrons

   J= /L+S/ …… /L-S/

The term symbol

The term symbol consists of

1. The state **L**
2. The multiplicity **(2S+1)**
3. **J value** $^{(2S+1)}L_J$

They specified as
L value gives the type of state as shown below
State
L=0 → **S**
L=1 → **P**
L=2 → **D**
L=3 → **F**
L=4 → **G**
$\mathbf{J = |L+S| \ldots . |L-S|}$

When the orbital is more than half filled the highest value of J is taken , and when it is less than half filled lower value of J is taken . when the orbital is half filled there is only one value of J.

Filled orbitals do not taken under consideration because in such orbitals **L=0,S=0 & J=0**

So the term symbols is ^{1}**S**

Exercises

1. Write the term symbols for the following atoms and ions in their ground states.

$_7$**N**, $_{17}$**Cl**, $_{11}$**Na**, $_{26}$**Fe**, $_{27}$**Co**$^{3+}$, $_{25}$**Mn**, **Mn**$^{+4}$, $_{29}$**Cu**, $_{24}$**Cr**

$_7$**N** **1s**^{2} **2s**^{2} **2p**^{3}

+1	0	-1
1	1	1

L=(1*1)+(0*1)+(-1*1)=0 ∴ S state

$$\mathbf{s = \frac{n}{2}}$$ number of single electrons

$$\mathbf{s = \frac{3}{2}}$$

$2S+1= 2\frac{3}{2}+1=4$

$J=|L+S|\ldots.|L-S|$

$=\left|0+\frac{3}{2}\right|\ldots.\left|0-\frac{3}{2}\right|={}^{3}/_{2}$

∴ The term symbol for N-atom in its ground state is $^{4}S_{3/2}$

2. $_{17}$**Cl [Ne] 3s^{2} 3p^{5}**

L=(2*1)+(2*0)+(1*-1)=2+0-1=1 ∴ p-state

$S=\frac{n}{2}=\frac{1}{2} \qquad 2S+1=2*\frac{1}{2}+1=2$

$J=\left|1+\frac{1}{2}\right|\ldots.\left|1-\frac{1}{2}\right|$

$= \quad \frac{3}{2} \qquad \frac{1}{2}$

Term symbol $^{2}P_{3/2}$

$_{11}$**Na 1s^{2} 2s^{2} 2p^{6} 3s^{1}**

L=1*0=0 ∴ **S- state**

$S=\frac{n}{2}=\frac{1}{2}$

$J=|L+S|\ldots.|L-S|$

$=\left|0+\frac{1}{2}\right|\ldots.\left|0-\frac{1}{2}\right|$

$= \quad \frac{1}{2} \qquad \frac{1}{2}$

$2S+1=2*\frac{1}{2}+1=2$

The term symbol for Na is $^{2}S_{1/2}$

$_{26}$**Fe[Ar] 4s^{2} 3d^{6}**

↑⇂		↑⇂	↑	↑	↑	↑

L=(2*+2)+(1*+1)+(1*0)+(1*-1)+(1*-2)

= 4+1+0-1-2=2 ∴ **D** state

$S=\frac{n}{2}=\frac{4}{2}=2$

$J=|L+S|\ldots.|L-S|$

$= \; |2+2| \ldots . |2-2|$

$= \quad 4 \qquad\qquad 0$

2S+1=2*2+1=5 the term symbol $^5D_4$

$_{27}Co^{+3}$

$_{27}Co[Ar]4s^2\,3d^7$

$Co^{+3}[Ar]4s^0\,3d^6$

	+2	+1	0	-1	-2
	1⇂	1	1	1	1

L=(2*2)+(1*1)+(1*0)+(1*-1)+(1*-2)

=4+1+0-1-2=2 ∴ **D** - state

$S = \frac{4}{2} = 2$

J= $|2+2| \ldots . |2-2|$

$4 \qquad\qquad 0$

2S+1=2*2+1=5 $^5D_4$

$_{25}Mn[Ar]\,4s^2\;\;3d^5$

	+2	+1	0	-1	-2
1⇂	1	1	1	1	1

L=(1*+2)+(1*+1)+(1*0)+(1*-1)+(1*-2)

=2+1+0-1-2=0 ∴ **S** – state

$$S = \frac{n}{2} = \frac{5}{2}$$

$J = |L+S| \ldots . |L-S|$

$= \; |0+5/2| \ldots . |0-5/2|$=5/2

2S+1=2*$\frac{5}{2}$+1=6 $^6S_{5/2}$

$Mn^{+4}\,[Ar]\,4s^0\;\;3d^3$

	+2	+1	0	-1	-2
	1	1	1		

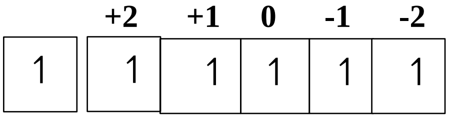
L=(1*(+2)) +(1*(+1)) +(1*0)=3 **∴ F-state**

$$s = \frac{n}{2} = \frac{3}{2}$$

$$J = |3 + 3/2| \ldots . |3 - 3/2|$$

= 9/2 3/2 **$^4F_{3/2}$**

$_{24}$Cr [Ar] $4s^1$ $3d^5$



L= (1*0)+(1*+2)+(1*+1)+(1*0)+(1*-1)+(1*-2)

= 0+2+1+0-1-2=0 **∴ S – state**

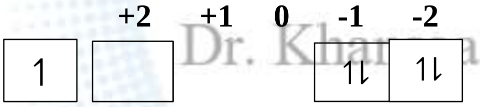
$$S = \frac{n}{2} = \frac{6}{2} = 3$$

$$J = |0 + 3| \ldots . |0 - 3| = 3$$

2S+1=2*3+1=7 **$^7S_3$**

For Cr^{+1} ? Cr^{+1} [Ar] $4s^0$ $3d^5$ **H.W**

$_{29}$Cu [Ar] $4s^1$ $3d^{10}$



L=(1*0)+(2*+2)+(2*+1)+(2*0)+(2*-1)+(2*-2)

= 0+4+2+0-2-4=0 **∴ S-state**

$$S = \frac{1}{2}$$

$$J = \left|0 + \frac{1}{2}\right| \ldots . \left|0 - \frac{1}{2}\right|$$

$$= +\frac{1}{2} \qquad +\frac{1}{2}$$

2S+1=2*$\frac{1}{2}$+1=2 **∴ $^2S_{1/2}$**

Exercise 2

1. Show that **s^1** configuration corresponds to **$^2S_{1/2}$** term symbol

S^1 m$_\ell$=0

1

$\therefore$ **L=1*0 =0** $\therefore$ **S** – state

$$\mathbf{S=\frac{n}{2}=\frac{1}{2}}$$

$$\mathbf{J=\left|0+\frac{1}{2}\right|....\left|0-\frac{1}{2}\right|}=\frac{1}{2}$$

2S+1=2*$\frac{1}{2}$+1=2 $\therefore$ **$^2S_{1/2}$**

2. Show that **d^1** configuration corresponds to term symbol **$^2D_{3/2}$**

d^1

+2	+1	0	-1	-2
1				

L=1*+2=2 $\therefore$ **D** – state

$$\mathbf{S=\frac{1}{2}}$$

$$\mathbf{J=\left|2+\frac{1}{2}\right|....\left|2-\frac{1}{2}\right|}$$

= **5/2** **3/2**

2S+1=2*$\frac{1}{2}$+1=2 $\therefore$ **$^2D_{3/2}$**

Exercise 3

Write the orbital classification which leads to the following ground terms:

$^4S_{3/2}$ $^2P_{3/2}$ $^3P_0$ $^4F_{3/2}$

1. $^4S_{3/2}$

2S+1=4 ; $\mathbf{S=\frac{3}{2}}$ $\therefore$**3 une**

S – state means L=0

$$\mathbf{J=|0+3/2|....|0-3/2|=3/2}$$

.. one value for J $\therefore$ the orbital is half filled

$\therefore$ P-orbital; orbital classification is **P^3**

1	1	1

2. $^{2}P_{3/2}$

$$2S+1=2\ ;\quad S=\frac{1}{2}$$

P- state L=1

$$J=\left|1+\frac{1}{2}\right|\ldots.\left|1-\frac{1}{2}\right|$$

= 3/2 1/2

Orbital classification is **P^5**

1⇂	1⇂	1

3. $^{3}P_{0}$

$$2S+1=3\ ;\ S=\frac{2}{2}=1$$

P-state L=1

$$J=|1+1|\ldots.|1-1|$$

2 0

$\therefore {}^{2}P$

1	1	

4. $^{4}F_{3/2}$

$$2S+1=4\ ;\ S=\frac{3}{2}$$

L=3 ∴ d-orbital

$$J=|3+3/2|\ldots.|3-3/2|$$

= 9/2 3/2

$\therefore d^3$

+2	+1	0	-1	-2
1	1	1		

Term symbols for excited states

In excited states the electrons could occupying any orbital even they can change their spins

E.g: carbon atom in it's excited state the P^2 electrons can occupying different orbitals and changing spins.

$_{6}C\ \ 1s^2\,2s^2\,2p^2$

↿	**↿**		**↿**		**↿**	**↿**		**↿**	Parallel spins
⇂	⇂		⇂		⇂	⇂		⇂	
↿⇂				↿⇂				↿⇂	opposite spins
↿	⇂		↿		⇂		↿	⇂	
⇂	↿		⇂		↿		⇂	↿	

∴ there are **15** excited states they called the micro states.

∗ How to find the term symbols of these states and which term is the most stable?

m_ℓ									
-1		↑	↑			↓		↓	↑↓
0	↑		↑		↓		↑↓	↑	
+1	↑	↑		↑↓	↑	↑			
L	**+1***	**0***	**-1***	**+2**	**+1**	**0**	**0**	**-1**	**-2**

^{3}P **^{1}D** **^{1}S**

∴ The term symbols for carbon atom or P^2 electronic configuration in excited states are ^{3}P ^{1}D ^{1}S

The most stable state is that of the highest value of multiplicity (2S+1) so ^{3}P state is most stable state. If multiplicity is equal a state of the highest value of L is the most stable one , so $^1D > {}^1S$

If we rank the above states according to their stability they become as:

$^3P > {}^1D > {}^1S$

← Stability increase

Ex: What are the term symbols that will be arised for V^{+3} ion in excited states.

$_{23}$V [Ar] $4s^2$ $3d^3$
V^{+3} [Ar] $4s^0$ $3d^2$

1. Parallel spins

mℓ										
-2				↑			↑		↑	↑
-1			↑			↑		↑		↑
0		↑			↑			↑	↑	
+1	↑				↑	↑	↑			
+2	↑	↑	↑	↑						
L	**+3***	**+2***	**+1***	**0***	**+1**	**0**	**-1**	**-1***	**-2***	**-3***

^{3}F **^{3}P**

2. Opposite spins

mℓ															
-2					↓				↓			↓		↓	↑↓
-1				↓				↓			↓		↑↓	↑	
0			↓				↓			↑ ↓	↑	↑			
+1		↓				↑↓	↑	↑	↑						
+2	↑↓	↑	↑	↑	↑										
L	**+4***	**+3***	**+2***	**+1***	**0***	**+2**	**+1**	**0·**	**-1**	**0**	**-1***	**-2**	**-2***	**-3***	**-4***

^{1}G **^{1}D** **^{1}S**

^{3}F > ^{3}P > ^{1}G > ^{1}D > ^{1}S

←

Stability increase

How to find the number of microstates for any electronic configuration, it could be achieved by using the following expression:

Number of microstates **(M.st)=** $\frac{n!}{r!(n-r)!}$

n= number of orbitals **x$_2$** **i.e** **n= (2ℓ+1)2**.

r= number of electrons

! factorial

Eg: calculate the number of microstates for $_{8}$**O-**atom (or $\mathbf{P^4}$ electronic configuration)

$\mathbf{_{8}O\ \ 1s^2\ \ 2s^2\ \ 2p^4}$

$\therefore \mathbf{M.st} = \frac{n!}{r!(n-r)!}$

for P-orbital **n=6** because $\mathbf{(2\ell+1)2=(2*1+1)2}$

r=4 **=6**

$\therefore \mathbf{M.st} = \frac{6!}{4!(6-4)!} = \frac{6!}{4!(2)!} = \frac{6*5*4!}{4!(2*1)} = \frac{30}{2} = 15$

For C-atom or $\mathbf{P^2}$ configuration

$\mathbf{_{6}C\ \ 1s^2\ \ 2s^2\ \ 2p^2}$

For P-orbital n= 6 because (2 ℓ + **1)2 = (2 × 1+1)2= 6**

r= 2

$\mathbf{M.st} = \frac{6!}{2!(6-2)!} = \frac{6!}{2!(4)!} = \frac{6*5*4!}{2*1*4!} = \frac{30}{2} = 15$

For $\mathbf{_{21}Sc\ [Ar]\ \ 4s^2\ \ 3d^1}$

n for d- orbital=**10**

$$\mathbf{M.st} = \frac{10!}{1!(10-1)!} = \frac{10*9!}{1*1(9)!} = \frac{10}{1} = 10$$

for $\mathbf{Cu^{+1}}$ **ion**

$\mathbf{_{29}Cu\ [Ar]\ 4s^1\ \ 3d^{10}}$

$\mathbf{Cu^{+}[Ar]\ 4s^0\ \ 3d^{10}}$

$$\mathbf{M.st} = \frac{10!}{10!(10-10)!} = \frac{10!}{10!(0)!} = \frac{10!}{10!*1} = 1$$

For $\mathbf{Cu^{+2}}$ **ion**

$\mathbf{Cu^{+2}\ 4s^0\ \ 3d^9}$

$\mathbf{M.st} = \frac{10!}{9!(10-9)!} = \frac{10*9!}{9!(1)!} = \frac{10}{1} = 10$

$\therefore\ \ \mathbf{d^1 \equiv d^9}$

For Ti atom

$\mathbf{_{22}Ti\ [Ar]\ \ 4s^2\ \ 3d^2}$

$\therefore \mathbf{d^2}$ **confg.**

$$\mathbf{M.st} = \frac{\mathbf{10!}}{\mathbf{2!\,(10-2)!}} = \frac{\mathbf{10 * 9 * 8!}}{\mathbf{2 * 1(8)!}} = \mathbf{45}$$

For $_{28}$**Ni-atom**

$_{28}$Ni [Ar] $4s^2$ $3d^8$

∴ **d^8 confg**

$$\mathbf{M.st} = \frac{\mathbf{10!}}{\mathbf{8!\,(10-8)!}} = \frac{\mathbf{10 * 9 * 8!}}{\mathbf{8!\,(2!)}} = \mathbf{45}$$

∴ **$d^2 \equiv d^8$**

We conclude that :

d^n configuration	number of microstates
d^1 d^9	**10**
d^2 d^8	**45**
d^3 d^7	**120**
d^4 d^6	**210**
d^5	**252**
d^{10}	**1**

Shelding and effective Nuclear charge:

An electron in a higher energy level is (screened) from seeing **100%** (all the protons) of the nuclear charge by the electrons in lower energy levels. We usually talk about the valence electrons and how they are screened from experiencing the complete nuclear charge. This screening depends on the sublevel (orbital type) occupied by the electron being screened.

The "Effective Nuclear Charge" is the nuclear charge that an electron experiences when other electron "screen" the nuclear charge.

Zeff or $\overset{*}{Z} = Z - S$

effective nuclear charge

atomic number (nuclear charge)

Shelding constant

Slater's Rules:

1- Write out the electronic configuration of the element in the following order and grouping **(1s) (2s 2p) (3s 3p) (3d) (4s 4p) (4d) (4f) (5s 5p)**.

2- Electrons for which the principle quantum number **(n)** is larger than the value of **(n)** for the electron of interest contribute zero to the value of **S**.

3- Consider a particular electron in an **(ns)** or **(np)** orbital.

- **i-** Each of other electrons in the **(ns/np)** group contributes. **S = 0.35**
- **ii-** Each of the electrons in the **(n-1)** shell contributes. **S = 0.85**
- **iii-** Each of the electrons the **(n-2)** or lower shells contributes **S = 1.00**

4- Consider a particular electron in the **(nd** or **nf)** orbital.

- **i-** Each of the other electrons in the **(nd nf)** group contributes **S = 0.35**
- **ii-** Each of the electrons in lower group than the one being considered. **S = 1.00**

Eg.1/ Calculate the effective nuclear charge that is exhibited by the valance electron of **(k)** atom.

K_{19}: $1s^2\ \ 2s^2\ \ 2p^6\ \ 3s^2\ \ 3p^6\ \ 4s^1$

$(1s^2)\ (2s^2\ 2p^6)\ (3s^2\ 3p^6)\ (4s^1)$

n-2 n-1 n

$S = 0 \times 0.35 + 8 \times 0.85 + 10 \times 1 = 16.8$

$\overset{*}{Z} = Z - S$

$= 19 - 16.8 = 2.2$

Eg 2/ Calculate the effective nuclear charge that is exhibited by:

1- The valance electron of **(Cu)** atom and **2-** for electron **(d)** in the same atom

Cu_{29}: $1s^2\ \ 2s^2\ \ 2p^6\ \ 3s^2\ \ 3p^6\ \ 4s^1\ \ 3d^{10}$

$(1s^2)\ \underset{n-2}{(2s^2\ 2p^6)}\ \underset{n-1}{(3s^2\ \ 3p^6\ \ 3d^{10})}\ \underset{n}{(4s^1)}$

$S = 0 \times 0.35 + 18 \times 0.85 + 10 \times 1 = 25.3$

$\therefore \overset{*}{Z} = 29 - 25.3 = 3.7$

2- For electron **(d)**

3- $(1s^2)\ (2s^2\ \ 2p^6)\ (3s^2\ \ 3p^6\ \ 3d^{10})\ (4s^1)$

$\therefore S = 9 \times 0.35 + 18 \times 1 = 21.15$

$\therefore \overset{*}{Z} = 29 - 21.15 = 7.85$

Eg. 3/ Estimate values of $\overset{*}{Z}$ for:

a- (4s) and **b- (3d)** electron in **(V)** atom

V_{23}: $1s^2\ \ 2s^2\ \ 2p^6\ \ 3s^2\ \ 3p^6\ \ 4s^2\ \ 3d^3$

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

$S = 1 \times 0.35 + 11 \times 0.85 + 10 \times 1 = 19.7$

$\therefore \overset{*}{Z} = 23 - 19.7 = 3.3$

b- $1s^2\ (2s^2\ \ 2p^6)\ (3s^2\ \ 3p^6\ \ 3d^3)\ (4s^2)$

$S = 2 \times 0.35 + 18 \times 1 = 18.7$

$\overset{*}{Z} = 23 - 18.7 = 4.3$

Problems:

Solve the following problems and give conclusions

Rank the following isoelectronic species according to the order of increasing in their size

a- Na^+ Ne F^-

b- Ar^+ K Cl^-

c- Sc^{+3} Ar Ca^{+2}

Since the species are isoelectronic so they possess the same electronic configuration.

a- $\mathbf{Na^{+}}$ **Ne** $\mathbf{F^{-}}$

$\mathbf{1s^{2}\ \ 2s^{2}\ \ 2p^{6}}$

$\mathbf{S = 7 \times 0.35 + 2 \times 0.85 = 4.15}$

$\mathbf{\overset{*}{Z}\ Na^{+} = Z - S = 11 - 4.15 = 6.85}$

$\mathbf{\overset{*}{Z}\ Ne = Z - S = 10 - 4.15 = 5.85}$

$\mathbf{\overset{*}{Z}\ F^{-} = Z - S = 9 - 4.15 = 4.85}$

$\mathbf{F^{-} > Ne > Na^{+}}$

As $\overset{*}{Z}$ increase the size of atom or ion decrease.

b- **Ar** $\mathbf{K^{+}}$ $\mathbf{Cl^{-}}$ electronic configuration

$\mathbf{1s^{2}\ \ 2s^{2}\ \ 2p^{6}\ \ 3s^{2}\ \ 3p^{6}}$

c- $\mathbf{Sc^{+3}}$ **Ar** $\mathbf{Ca^{+2}}$ electron configuration

$\mathbf{1s^{2}\ \ 2s^{2}\ \ 2p^{6}\ \ 3s^{2}\ \ 3p^{6}}$

In isoelectronic species (ion, atom) that have the same electronic configuration

$\overset{*}{Z}$ increase as atomic number **(Z)** increase and the value of shelding constant is the same. As atomic number **Z** increase the size of species decrease in

b- $\mathbf{{}_{17}Cl^{-} > {}_{18}Ar > {}_{19}K^{+}}$

c- $\mathbf{{}_{18}Ar > {}_{20}Ca^{+2} > {}_{21}Sc^{+3}}$

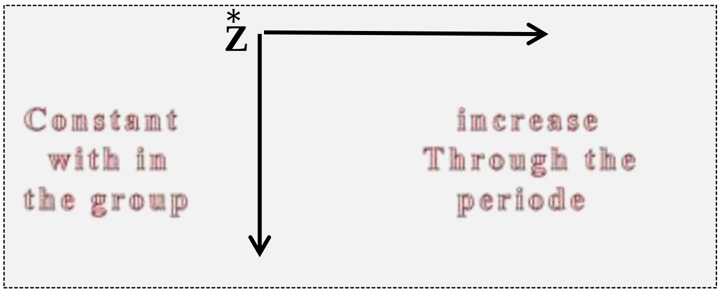
$$\therefore \overset{*}{Z} \propto \frac{1}{size}$$

Effect of $\overset{*}{Z}$ in atomic properties

The atomic properties like:

atomic size, ionic size, ionization energy affected by the value of $\overset{*}{Z}$

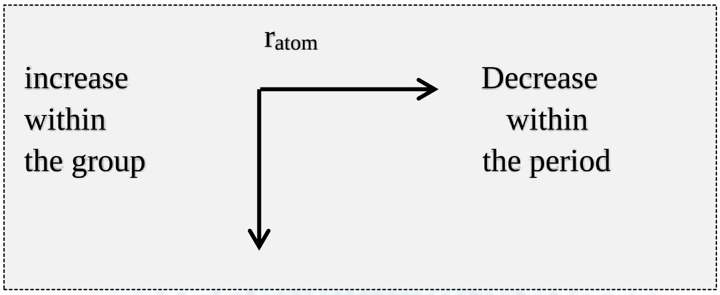
Trend in $\overset{*}{Z}$



1- Atomic size (Atomic Radius):

Since atoms are spherically symmetrical so the could be expressed by their radii (r_{atom}).

r_{atom}: the distance between the two nuclie of two adjacent atoms in the element divided by two.



Q1\ Why Atomic radii decrease through the period?

From left to right **Zeff** increases as we add electron to the same energy level n is constant. The nuclear charge as we move across a period is not completely screened by the additional valence electrons so **Zeff** becomes large for each valence electron $\therefore \overset{*}{Z} \propto \frac{1}{r_{atom}}$

Q2\ Why atomic radii increase down a group?

As we move down a group **(n)** increases for the valance electrons, hence the orbital size also in increases **Zeff** also increases **(sligtly)**, but the valence electron spend more time further from the nuclear in the large orbitals.

There is a sharp increase in atomic radii in the beginning of each new period followed by gradual decrease as a result of sharp increasing in **(n)** with decreasing in $\overset{*}{Z}$. see Fig. (6).

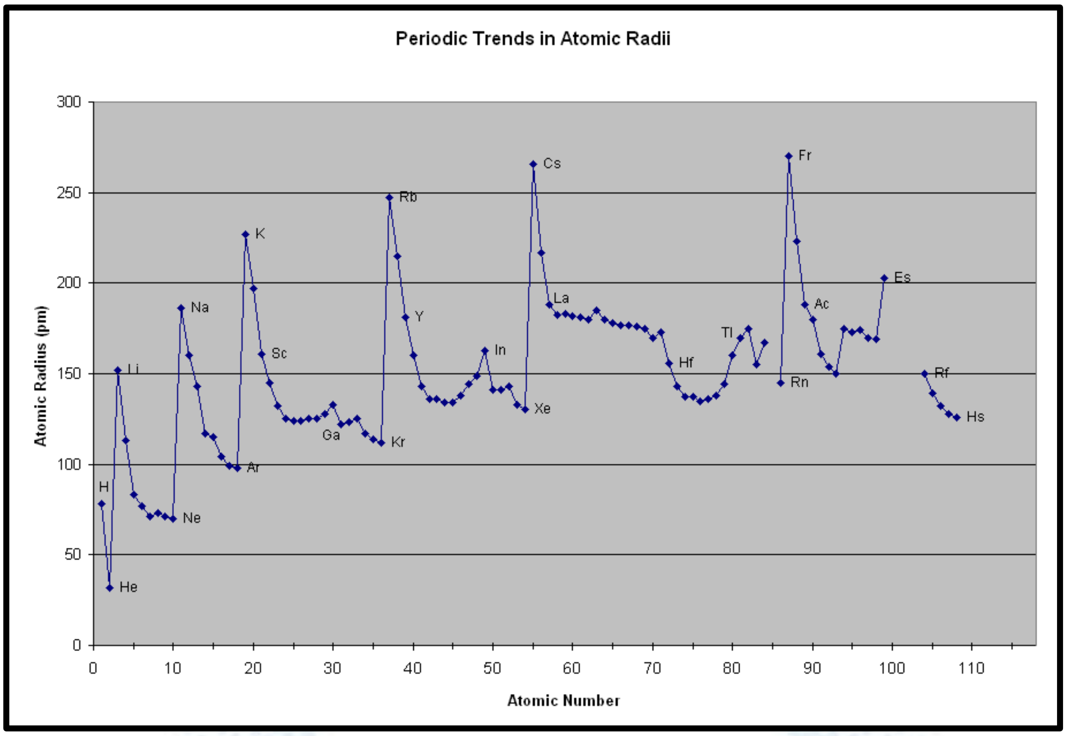


Fig. (2)

2. Ionization Potential, I.P or Ionization Energy IE.

Is the energy needed to remove an outer electron from an atom in the gas phase to make a positive ion $\mathbf{M_{(g)}} \longrightarrow \mathbf{M^{+}_{(g)}} + \mathbf{e^{-}}$

Each atom can have a series of ionization to produce a multi-charge cation.

For example consider the ionization of **Mg(g)**:

1- First: $\mathbf{Mg_{(g)}} \longrightarrow \mathbf{Mg^{+}_{(g)}} + \mathbf{e^{-}}$ $\mathbf{IE_1 = +738KJ/mol}$

2- Second: $\mathbf{Mg^{+}_{(g)}} \longrightarrow \mathbf{Mg^{+2}_{(g)}} + \mathbf{e^{-}}$ $\mathbf{IE_2 = +1451\ KJ/mol}$

3- Third: $\mathbf{Mg^{+2}_{(g)}} \longrightarrow \mathbf{Mg^{+3}_{(g)}} + \mathbf{e^{-}}$ $\mathbf{IE_3 = +7733\ KJ/mol}$

∴ it is (endo thermic reacation) **I.P** is measured by **eV**, KJ/mol, kcal/mol

- Why the **I.E** increase from $\mathbf{I.E_1}$ to $\mathbf{I.E_2}$ **?**

  I.P increase as oxidation state of cation increase, because it is more difficult to remove an electron from positive ion so:

  $\mathbf{I.E_1 < I.E_2 < IE_3}$

  I.P or **I.E** data indicate

***** Atoms with low **I.P** tend to form cations during chemical reactions show basic properties act as reducing agents and have metallic properties (eg: group **1**) (electrons alkali metals)

***** Atoms with high **I.P** tend to form anion during chemical reaction show acidic properties act as oxidizing agents and non-metalic properties (eg: halogens group **17**).

***** The I.P values give indication about the number of valence electrons in the outer shell so the element could be identified from these informations

Eg: Name the (period **3**) element with the following **I.P** in **KJ/mol** and with its electronic configuration

$I.P_1$	$I.P_2$	$I.P_3$	$I.P_4$	$I.P_5$	$I.P_6$
1012	**1903**	**2900**	**4956**	**6278**	**22230**

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

high jump in $I.P_6$ belongs to the closed shell (**n = 2**)

∴ the element have (**15**) electron ∴ **p** **the element is phosphorus**

Eg: Calculat the high jump for (**Na**)

$_{11}Na : 1s^2\ \ 2s^2\ \ 2p^6\ \ 3s^1$

∴ high jump for **Na** = (oxidation statetl) **= 1+ 1 ⇒** $I.P_2$

H.W1/ Name the element **X** in the period **3** that has the following **I.P** in **KJ/mol**

2/ Caculat the atomic number and write the electronic configuration for the element **X** in the period **3** that has the following **I.P in KJ/mol and name the element.**

$I.P_1$	$I.P_2$	$I.P_3$	$I.P_4$	$I.P_5$	$I.P_6$
577	**1816**	**2744**	**11576**	**14829**	**18375**

3/ Why $_{12}Mg$ have (High jump) from $I.P_2$ to the $I.P_3$**?**

3. Factors affecting I.P

1- Distance between the outer most shell electron and the mucleous (r_{atom} or r_{ion}). As this distance increase **I.P decrease** because: the electron being loosely held by the nucleous.

2- The effective nuclear charge ($\overset{*}{Z}$) as electron is strongly held by the nucleous so the atomic or ionic size reduced.

3- Type of subshell from which the leaving electron belongs which depends on the penetrating ability of the orbital.

$\therefore s > p > d > f$ $\xleftarrow{\hspace{3cm}}$

More difficult to leave the electron

Eg/ I.P₁ for **Be = 9.3 eV**; **I.P₁** for **B = 8.3 eV**

$_4\mathbf{Be}\ \ 1s^2\ \ 2s^2 \xrightarrow{9.3\ eV} \mathbf{Be}^+$; $_5\mathbf{B}\ \ 1s^2\ \ 2s^2\ \ 2p^1 \xrightarrow{8.3\ eV} \mathbf{B}^+$

because/ s-electron must be removed	**s > p**	p-electron must be removed

4- Completely filled and half filled orbital According to Hund's rule atoms having half filled or completely filled orbitals are more stable and hence more energy is needed to remove an electron from such atoms. The **I.P** of such atoms is therefore higher than expected from their position in periodic table.

Eg/ I.P₁ of (**N**) > **I.P₁** of (**O**)

$\mathbf{N}_7\ \ 1s^2\ \ 2s^2\ \ 2p^3$ $\quad$ $_8\mathbf{O}\ \ 1s^2\ \ 2s^2\ \ 2p^4$

↿	↿	↿

⇅	↿	↿

half filled orbital more stable higher energy is required to remove an electron	less stable lower energy is required to remove an electron

5- The charge of ion (oxidation number), the increasing in loosing electrons lead to decrease in (**S**) value, so $\overset{*}{\mathbf{Z}}$ increase and $\mathbf{r}^+$ decrease, which results the remaining electrons strongly held by the nucleus so **I.P** increase

Q/ Why the cation's are smaller than atoms they came from?

or/ Why $\mathbf{r_{Na^+}} < \mathbf{r_{Na}}$

Q/ why the an ions are larger than atoms they come from?

or/ why $\mathbf{r_{F^-}} > \mathbf{r_F}$

Trend of I.P$_1$

1) **I.P$_1$** decrease down the group since (r_{atom}) increase in this trend and $\overset{*}{\mathbf{Z}}$ is constant while (**n**) increase.
2) There is a sharp change in the value of **I.P$_1$** between the last element in the period and first element of the new period as in (**He** $\longrightarrow$ **Li**) and (**Ne** $\longrightarrow$ **Na**) due to the sharp change in atomic size.
3) Generally **I.P$_1$** increase through the period due to increase in $\overset{*}{\mathbf{Z}}$ in the same direction, But the increase is irregular when coming from group **2 + 12** to group **13** neighbour and from group **15** to group **16** neighbour,Fig.7.

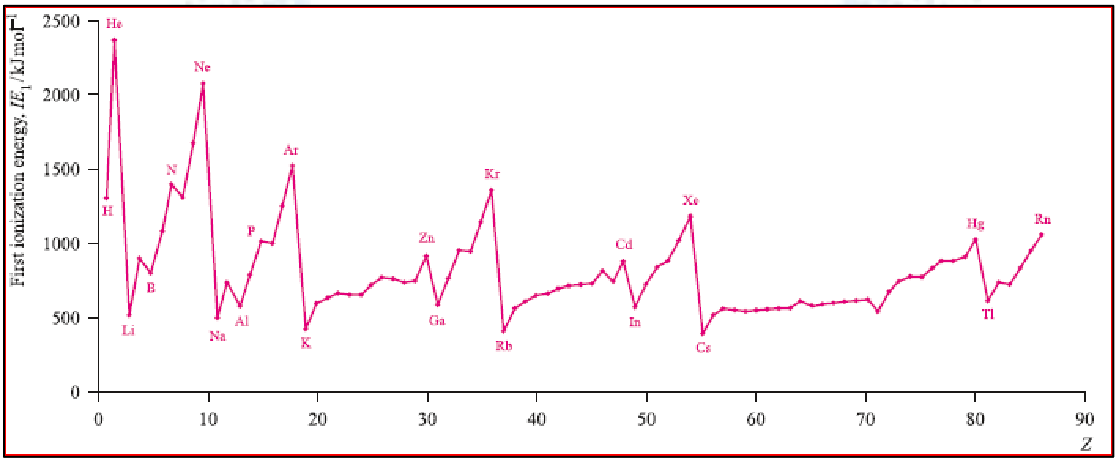


Fig.7 The values of the first ionization energies of the elements up to Rn.

Q/ Why **I.P$_1$** of **Be > B**

because the outer electron in ($_5$**B**) $\mathbf{1s^2}$ $\mathbf{2s^2}$ $\mathbf{2p^1}$ belongs to p-orbital while in ($_4$**Be**) $\mathbf{1s^2}$ $\mathbf{2s^2}$ the outer electron belongs to s-orbital so it is more difficult to remove.

Q/ Why **I.P$_1$** of **N > O**

($_7$N): $\mathbf{1s^2}$ $\mathbf{2s^2}$ $\mathbf{2p^3}$ because the electronic configuration (half filled orbitals) more stable.
∴ higher **I.P$_1$**
While $_8$O: $\mathbf{1s^2}$ $\mathbf{2s^2}$ $\mathbf{2p^4}$ electron configuration of the outer shell (more than half filled less stable, lower **I.P$_1$**)

Q/ Draw a diagram showing a change of **I.P$_1$** in the period (**2**), explaining the anomalous in some values.

4) Group **1** elements have the lowest values of **I.P$_1$**

While (group **18**) elements (noble gases) have the highest values of **I.P$_1$** because they all have high effective nuclear charge due to their octet formation and require a high amount of energy to destroy that stable configuration.

3. Electron affinity: (EA)

Is the energy released when an electron is added to neutral atom in the gas phase.

For example $\mathbf{X_{(g)} + e^- \longrightarrow X^-_{(g)}}$ $\mathbf{\Delta H = -ve}$

∴ Exothermic reaction

$\mathbf{F_{(g)} + e^- \longrightarrow F^-_{(g)}}$ **EA = -328 KJ/mol**

$\mathbf{N_{(g)} + e^- \longrightarrow N^-_{(g)}}$ **EA > 0 KJ/mol**

First Electron affinity **EA$_1$** is <u>**negative value**</u> (exothermic reaction), But second **EA$_2$** is <u>**positive value**</u> (endothermic reaction), due to the repulsion between the negative ion and the electron so monovalent anions have **–ve EA**, while Divalent anions (**eg:** $\mathbf{O^{-2}}$, $\mathbf{S^{-2}}$) have +ve

$O(g) + e \longrightarrow O^{-}(g)$ EA1 = -143 KJ/mol

$\underline{O^{-}(g) + e \longrightarrow O^{-2}(g)}$ <u>EA2 = +782 KJ/mol</u>

$O(g) + 2e \longrightarrow O^{-2}(g)$ EA = +639 KJ/mol Total EA of oxygen

It is difficult to determine the electron affinity of the elements directly, it is determined experimentally through Born-Haber cycle (chapter **-3-**).

The following table show EA for some elements in KJ/mol

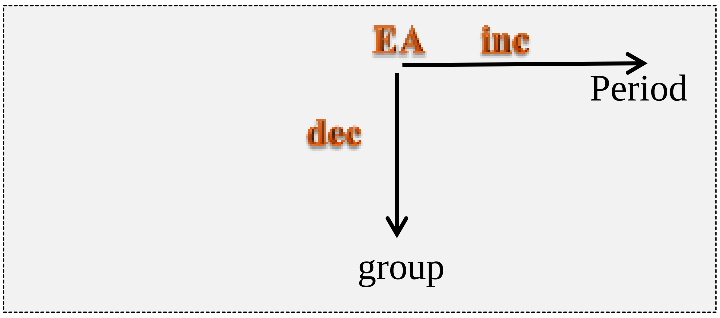
Element	**Anions**	**EA/KJmol^{-1}**
H	H^{-}	-72
F	F^{-}	-333
Cl	Cl^{-}	-364
Br	Br^{-}	-342
I	I^{-}	-295
O	O^{2-}	+639
S	S^{2-}	+390

Note/ all species (atom and ions) with completely filled outer shell have **EA = 0**

As shown from the table halogens (**G 17**) possess the highest **EA** values the most electronaffinity atom is (**Cl**) (not **F**) as expected. That is <u>due to small size</u> of °F-atom which leads to higher electronic repulsion of electron pairs

1- EA increase in period from left to right due to increase in $\overset{*}{Z}$ and decrease in atomic size and increase in I.P

2- EA decrease down if the group due to increase in atomic size and decrease in I.P



Q/ Why halogens possess the highest **EA** values?

That is due to:

1. The ease of gaining one electron to possess anobel gas configuration.

$_9F: 1s^2\ 2s^2\ 2p^5 \xrightarrow{+e} F^-: 1s^2\ 2s^2\ 2p^6 \equiv [Ne]$

2. The small atomic size of halogens as they liying at the end of each period
3. High value of $\overset{*}{Z}$

CHAPTER TWO

MOLECULES

Chapter Two

Molecules

Covalent Compounds:

General Properties:

1- Covalent Compounds are formed by the sharing of electrons between the atoms they exist as individual molecules held together by weak Vander Waal's forces.

2- Sometimes infinite covalent structures in three-dimensions (since covalent bond is directional) are formed rather than separated molecules, so there are strong forces in all directions, thus diamond and silica are covalent and have high melting points.

3- They may be solids, liquids or gases, their melting and boiling points are low.

4- They are generally soft, easily fusible and volatile.

5- They are generally soluble in organic solvents.

6- They can not carry electrical charges in all states so they act as insulator.

The Covalent Bond:

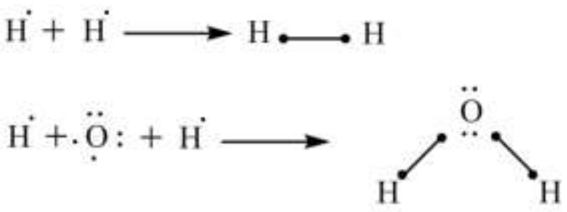
The foundation of modern chemical bonding theory were laid in **1916-1920** by Lewis and Langmuir, who suggested that ionic species were formed by electron transfer while electron sharing was important in covalent molecules. In some cases it was suggested that shared electron in a bond were provided by one of the atoms but that once the bond (sometimes called a coordinate bond) is formed.

In a covalent compounds, electrons are shared between atoms. In an ionic compounds, one or more electrons are transferred between atoms to form ions.

Types of Covalent Bonds:

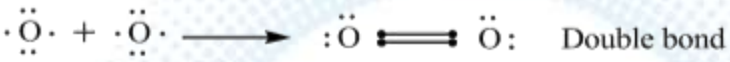
1- Single covalent bonds, are formed by sharing of only one electron pair between bonded atoms

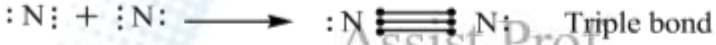
eg:



2- Double and Triple covalent bonds, are formed when the atoms bonded together share two or three electron pairs respectively

eg:





3- Other types of covalent bonds like, the polar covalent bond, coordination covalent bond and hydrogen bond.

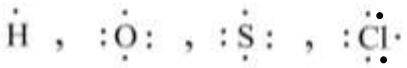
The Octet Rule:

An atom obeys the (Octet Rule) when it gains, loses or shares electrons to give an outer shell containing eight electrons (noble gas configuration) ($\mathbf{ns^2\ np^6}$).

Lewis Structures:

a) For atoms: a Lewis structure for an element consists of the element's symbol surrounded by dots that represent of valance electrons.

eg: Give Lewis electron dot structure for the following elements:
hydrogen, oxygen, sulphur, chlorine



b) For molecules and ions, like, H_2O, NH_3 , NH_4^+….. the following rules should be followed.

1- Determine the number of (total electrons) (**t**) of the molecule.

- **t = 2 for H**

  = 6 for B

  = 8 for all other elements.

2- Calculate the Valence electrons (**v**) for all atoms

- (the valance of each atom = it's group number)

eg: for **H = 1** for **B = 3** for **N = 5**

If you have anions add the number of **–ve** charges to (**v**), if you have cations subtract the number of **+ve** charges from (**v**).

3- After calculating (**t**) and (**v**) use the following formula to obtaine the number of bonding pairs of electrons **(b)**

$$b = \frac{t - v}{2}$$

4- Calculate the number of non bonding pairs (**n.b**) by the following formula

$$n.b = \frac{v - 2b}{2}$$

5- Determine the central atom in a molcule or ion

Note:

a) Oxygen can not be central atom only when it bond with **H**.

b) Carbon is the central atom in any compounds containing carbon, after determination of the central atom arrange the other atoms around it by using the number of (**b**) that calculated.

- In compounds containing **H** and **O** and third atom distribute the oxygen, around the central atom (avoid **O – O** bonds), and for most cases connect **H** to **O**

6- Fill the rest of structure with non bonding pair until (each hydrogen has two electrons), (each boron has six electrons) and other atoms has eight electrons.

7- Recheck to be sure that the total number of electrons shown in your structure equals (**v**).

Examples:

Write a Lewis dot structur for $\mathbf{NH_3}$ and $\mathbf{CO_3^{-2}}$

1- $\mathbf{NH_3}$

$\mathbf{t: 3H = 3 \times 2 = 6e}$

$\mathbf{1N = 1 \times 8 = \underline{8e}}$

$\mathbf{t = 14e}$

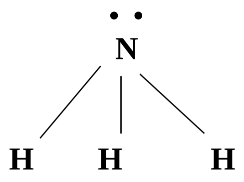
$\mathbf{v = 3H = 3 \times 1 = 3e}$

$\mathbf{1N = 1 \times 5 = \underline{5e}}$

$\mathbf{v = 8e}$

$\mathbf{b} = \frac{t - v}{2} = \frac{14 - 8}{2} = 3$ bonding pairs

$\mathbf{n.b} = \frac{v - 2b}{2} = \frac{8 - 6}{2} = 1$



2- $\mathbf{CO_3^{-2}}$

$\mathbf{t: 1C = 1 \times 8 = 8e}$

$\mathbf{3O = 3 \times 8 = \underline{24e}}$

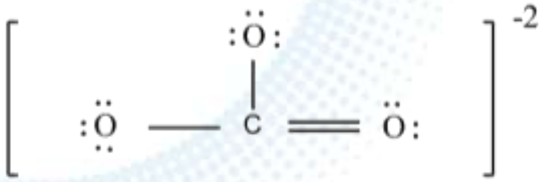
$\mathbf{t = 32e}$

$\mathbf{v: 1C = 1 \times 4 = 4e}$

$\mathbf{3O = 3 \times 6 = \underline{18e}}$

$\mathbf{v = 22}$

$\mathbf{v = 22 + 2e = 24e}$



$\mathbf{b} = \frac{32-24}{2} = 4$

$\mathbf{n.b} = \frac{24-8}{2} = 8$

H.W: Draw a Lewis structure for the following ions and molecules:

$[NH_4]^+$; H_3O^+, PCl_3, SO_4^{-2}, BF_3, HCN; H_2SO_4

Hybridization of Atomic Orbitals:

- **What is orbital Hybridization?**

Hybrid orbitals my be formed by mixing the characters of atomic orbitals that are close in energy. The character of a hybrid orbital depends on the atomic orbitals involved and their percentage contributions. The labels given to hybrid orbitals reflect the contributing atomic orbitals, **e.g.** an **sp** hybrid possesses equal amounts of **s** and **p** orbital character.

Hybrid orbitals are generated by mixing the characters of atomic orbitals.

sp Hybridization: it means that one **s** atomic orbital and one **p** atomic orbital mix to form a set of two hybrid orbitals with different direction properties. The model of **sp** hybridization can be used to describe the sigma bonding in a linear molecule such as **$BeCl_2$**.

sp^2 Hybridization: it means that one **s** and two **p** atomic orbitals mix to form a set of three hybrid orbitals with different directional properties. The model **sp^2** hybridization can be used to describe the sigma bonding in trigonal planar molecules such as **BH_3**.

sp^3 Hybridization: it means that one **s** and three **p** atomic orbitals mix to form a set of four hybrid orbitals with different directional properties. The model **sp^3** hybridization can be used to describe the sigma bonding in tetrahedral molecules such as **NH_3**

table (1): types of hybridization

Type of Hybridization	Shape	Bond angle	No. of hybrid orbitals
sp	**Linear**	**180°**	**2**
sp^2	**Trigonal planer**	**120°**	**3**
sp^3	**Tetrahedral**	**109°.28**	**4**
sp^3d	**Trigonal bipyramidal**	**120°**	**5**
sp^3d	**Square based pyramidal**	**90°**	**5**
sp^3d^2	**Octahedral**	**90°**	**6**
dsp^2	**Square planer**	**90°**	**4**

Examples:

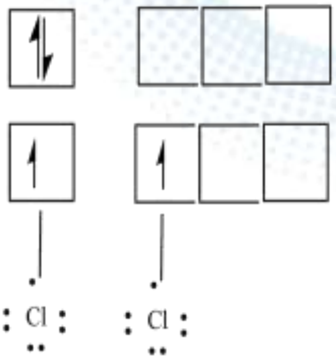
Find the type of hybridization of the central atom and the expected geometrical form with drawing of the following molecules:

$BeCl_2$, BCl_3, NH_3, C_2H_4, PF^-_6 , PCl_5

These hybridization and other types shown in table ( )

1) $BeCl_2$

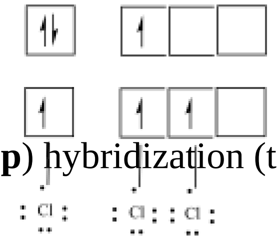
$_4Be$: $1s^2$ $2s^2$ $2p$ **$_{17}C1$: $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^5$**

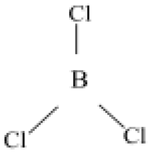


It is (**sp**) hybridization (Linear) **Cl – Be – Cl**

2) BCl_3

$_5B$: $1s^2$ $2s^2$ $2p^1$

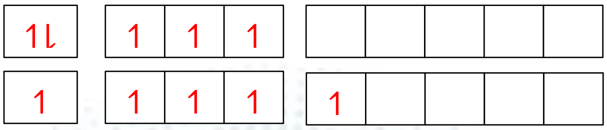


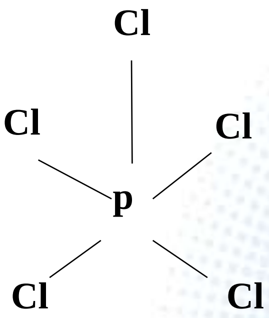


It is (**sp**) hybridization (trigonal planer)

3) PCl_5:

$_{15}P$: $1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^3$, $3d$

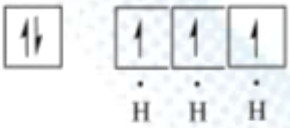


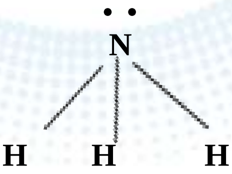


It is **(sp^3d)** hybridization (Trigonal bipyramidal)

4) NH_3

$_7N$: $1s^2$ $2s^2$ $2p^3$

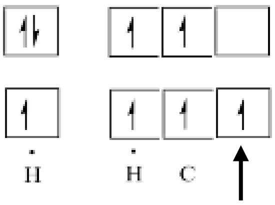


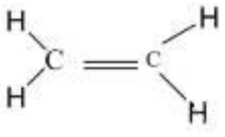


It is **(sp^3)** hybridization (Tetrahedral**)**

5) C_2H_4

$_6C$: $1s^2$ $2s^2$ $2p^2$



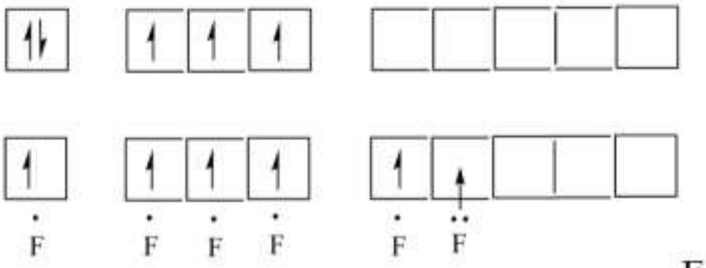


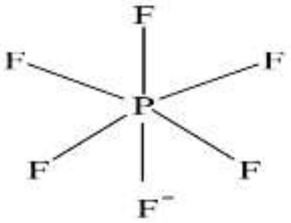
sp^2 hyperdization

excluded form hybridization to form π bond

6. $PF^-_6 \equiv PF_5F^-$

$_{15}P$: $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^3$ $3d$





It is **(sp^3d^2)** hybridization (Octahedral)

H.W. find the type of hybridization of the central atom and expected geometrical form with drawing of the following

H_2O, CO, $B_3N_3H_6$, $LiCH_3$

$B_3O_3(CH_3)_3$, NH^+_4, NH^-_2, C_6H_6,

[Be Cl_2 (OET_2)$_3$], $[BeF_4]^{-2}$,

[Be $(H_2O)_4]^{+2}$, H_3O^+, NF_3, H_2CO,

H_2S, SeF_6, $[SiF_6]^{-2}$, O_3, HCN, CS_2

Examples

Molecule	Geometry	hybridization
NH^{+}_{4} , NH_3 , $(NH_2)^-$	Tetrahedral	sp^3
NO_3 , NOCl	Trigonal planer	sp^2
N_2O	Linear	sp
$[PH_4]^+$, $SbCl_3$, PF_3, $POCl_3$	Tetrahedral	sp^3
$SbCl_5$, AsF_5 , PCl_5	Trigonal bipyramidal	sp^3d
$[AsF_6]^-$, $[PF_6]^-$, $[BiCl_6]^-$, $[SbF_5]^{-2}$	Octahedral	sp^3d^2
OH^{+}_{3}, H_2O	Tetrahedral	sp^3
SO_3, SO_2	Trigonal planer	sp^2
SO_2Cl_2, $SOCl_2$, SeO_4	Tetrahedral	sp^3
$TeCl_4$, SeF_4, SOF_4	Trigonal bipyramidal	sp^3d
TeF_6, SF_6, $[TeCl_5]^-$	Octahedral	sp^3d^2
IO^{-}_{4}, ClO^{-}_{4}, ClO^{-}_{2}, ICl^{+}_{2}	Tetrahedral	sp^3
$IO_2F^{-}_{2}$, ClF_3, ClF^{-}_{2}, BrF_3	Trigonal bipyramidal	sp^3d
$[IO_6]^{-5}$, IOF_5, IF_5, BrF_5	Octahedral	sp^3d^2

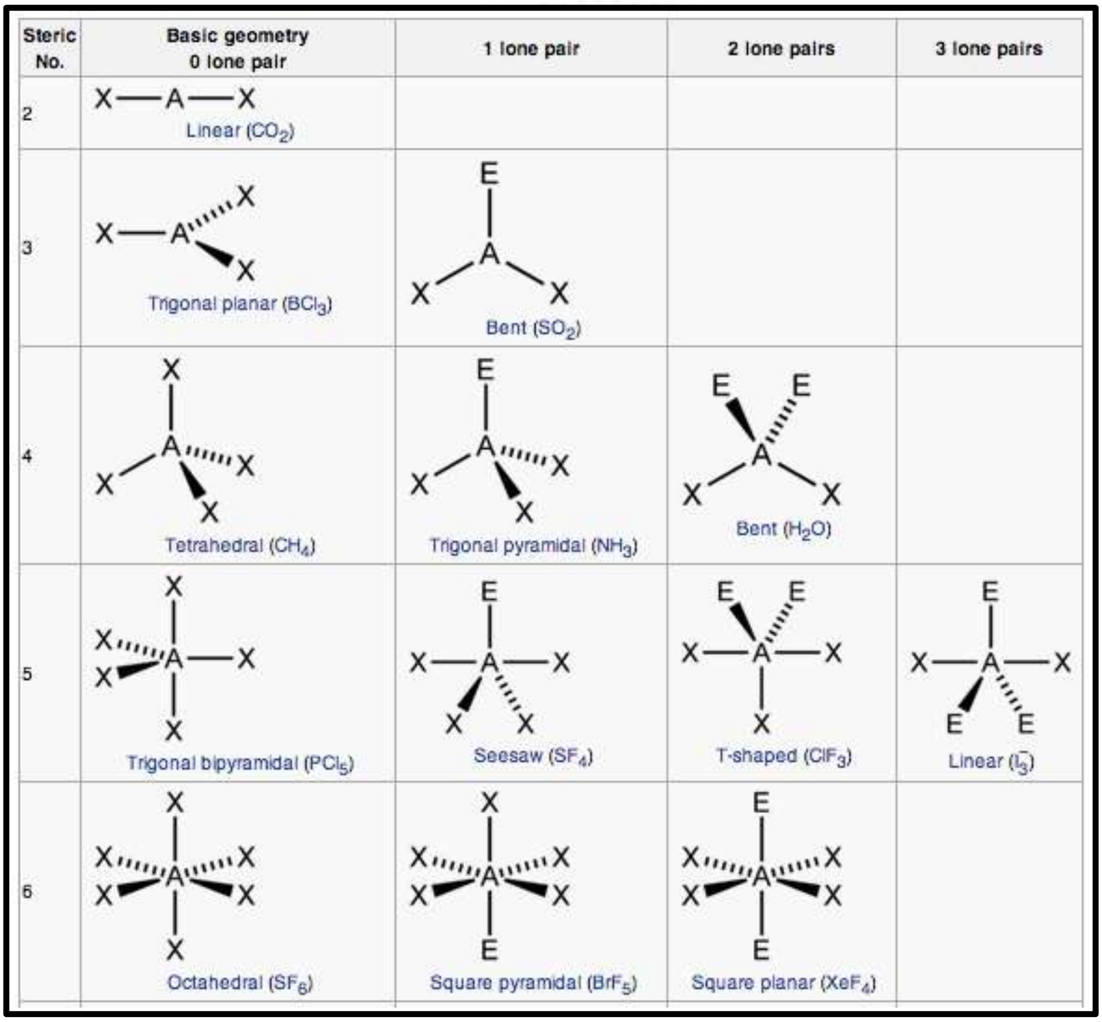
Valence Shell Electron Pair Repulsion theory (VSEPR) theory

VSEPR theory is a model used in chemistry to predict the geometry of individual molecules from the number of electron pairs surrounding their central atoms. It is also named the Gillespe-Nyholm theory.

The number of electron pairs in the valence shell of central atom is determined after drawing the Lewis structure of the molecule, and expanding it to show all bonding group and lone pairs of electrons. In VSEPR theory a double bond or triple bond are treated as a single bonding group.

AXE method:

The (**AXE**) method of electron counting is commonly used when applying the VSEPR theory. The electron pairs around a central atom are represented by a formula **AXnEm**, where Arepresented the central atom and always has an implied subscript one. Each **X** represent a ligand (an atom bonded to **A**). Each **E** represent a long pair of electrons on the central atom. The total number of **X** and **E** is Know the steric number. For example a molecule $\mathbf{AX_3E_2}$, the atom **A** has a steric number of **5**.



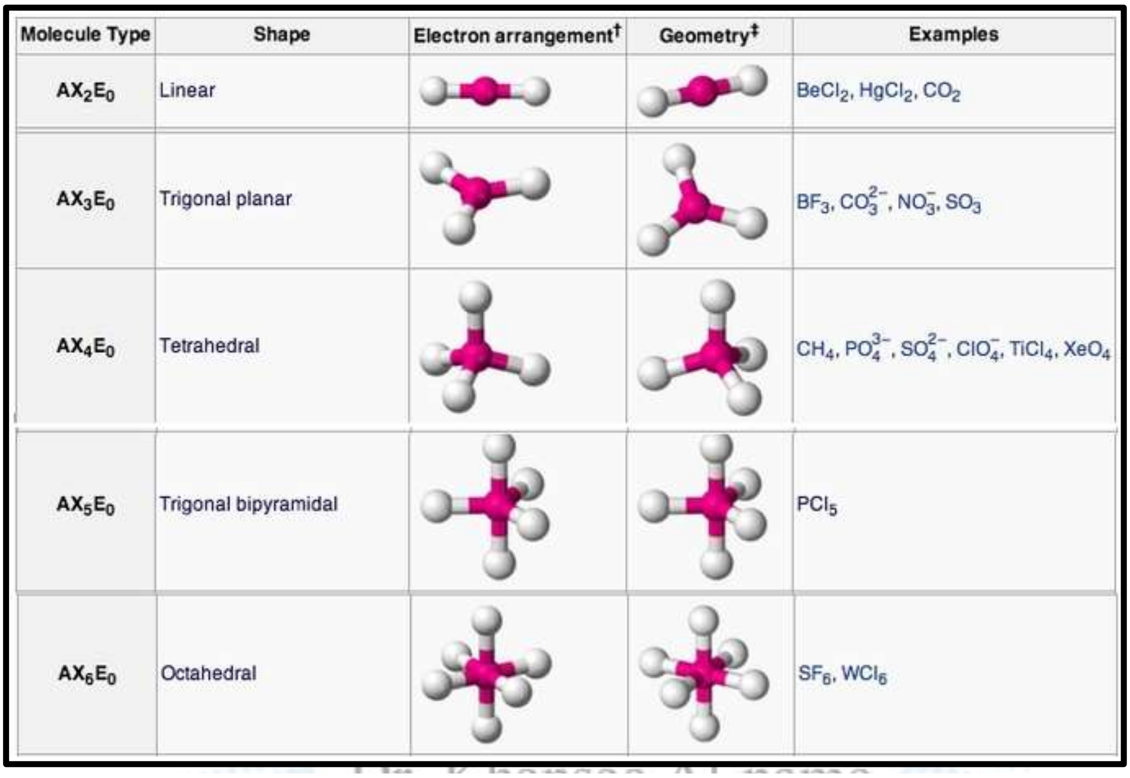
Steric No.	Basic geometry 0 lone pair	1 lone pair	2 lone pairs	3 lone pairs
2	Linear (CO_2)			
3	Trigonal planar (BCl_3)	Bent (SO_2)		
4	Tetrahedral (CH_4)	Trigonal pyramidal (NH_3)	Bent (H_2O)	
5	Trigonal bipyramidal (PCl_5)	Seesaw (SF_4)	T-shaped (ClF_3)	Linear (I_3^-)
6	Octahedral (SF_6)	Square pyramidal (BrF_5)	Square planar (XeF_4)	

AXE method:

The A represents the central atom; the X represents the number of sigma bonds between the central atoms and outside atoms; and the E represents the number of lone electron pairs surrounding the central atom.

The sum of X and E, known as the steric number, is also associated with the total number of hybridized orbitals used by valence bond theory.

Note that the geometries are named according to the atomic positions only, not the electron arrangement.



Molecule Type	Shape	Electron arrangement†	Geometry‡	Examples
AX_2E_0	Linear			$BeCl_2$, $HgCl_2$, CO_2
AX_3E_0	Trigonal planar			BF_3, CO_3^{2-}, NO_3^-, SO_3
AX_4E_0	Tetrahedral			CH_4, PO_4^{3-}, SO_4^{2-}, ClO_4^-, $TiCl_4$, XeO_4
AX_5E_0	Trigonal bipyramidal			PCl_5
AX_6E_0	Octahedral			SF_6, WCl_6

AXE method: annotation and examples: AXE annotation, geometry, and examples for each shape.

Main geometries (without lone pairs of electrons):

1. Linear

In a linear model, atoms are connected in a straight line, and a bond angle is simply the geometric angle between two adjacent bonds. A simple triatomic molecule of the type AX_2 has its two bonding orbitals 180° apart. Examples of triatomic molecules for which VSEPR theory predicts a linear shape include $BeCl_2$ (which does not possess enough electrons to conform to the octet rule) and CO_2. When writing out the electron dot formula for carbon dioxide, notice that the C-O bonds are double bonds; this makes no difference to VSEPR theory. The central carbon atom is still joined to two other atoms. The electron clouds that connect the two oxygen atoms are 180° apart.

Lewis dot structure of carbon dioxide:

Although the central atom (carbon) has four bonds, only two are sigma bonds; it is therefore is represented as AX_2E_0 in the table.

2. Trigonal planar

Molecules with the trigonal planar shape are triangular and in one plane, or flat surface. An AX_3molecule such as BF_3 has three regions of electron density extending out from the central atom. The repulsion between these will be at a minimum when the angle between any two is 120^o.

3. Tetrahedral

Tetra- signifies four, and -hedral relates to a face of a solid; “tetrahedral” literally means “having four faces. ” This shape is found when there are four bonds all on one central atom, with no lone electron pairs. In accordance with the VSEPR theory, the bond angles between the electron bonds are 109.5^o. An example of a tetrahedral molecule is methane (CH_4). The four equivalent bonds point in four geometrically equivalent directions in three dimensions, corresponding to the four corners of a tetrahedron centered on the carbon atom.

The lewis dot structure for methane:

The four hydrogen atoms are equidistant from each other, with all bond angles at 109.5°.

4. Trigonal bipyramidal

A trigonal bipyramidal shape forms when a central atom is surrounded by five atoms in a molecule. In the geometry, three atoms are in the same plane with bond angles of 120°; the other two atoms are on opposite ends of the molecule. Some elements in Group 15 of the periodic table form compounds of the type AX_5; examples include PCl_5 and AsF_5.

The Lewis dot structure of phosphorous pentachloride.:

The three equatorial atoms are in the same plane, with the two axial atoms located on opposite ends of the molecule.

5. Octahedral

Octa- signifies eight, and -hedral relates to a face of a solid, so "octahedral" literally means "having eight faces." The bond angles are all 90°, and just as four electron pairs experience minimum repulsion when they are directed toward the corners of a tetrahedron, six electron pairs try to point toward the corners of an octahedron. An example of an octahedral molecule (AX_6) is sulfur hexafluoride (SF_6).

CHAPTER THREE

MOLECULAR ORBITAL THEORY "MOT"

AO-AO interaction

Atomic orbital solutions derived from the Schrodinger wave equation, waves can be added together or subtracted from each other. The wave function describing a molecular orbital may be obtained by one of two ways:

1- Linear Combination of Atomic Orbitals **(L.C.A.O)**

2- United atom method.

L.C.A.O: MO arises from interactions between orbitals of atomic centers in the molecule and such interactions are:

1- allowed if symmetries of atomic orbitals are compatible with one another.

2- efficient if the region of overlap between the two atomic orbitals is significant.

3- efficient if the atomic orbitals are relatively close in energy.

When two atomic orbitals ovelap, they interact in two ways to form **2 (MO)** (a bonding molecular orbital) and an (anti bonding molecular orbital).

The first way:

Interact is (in-phase) which leads to an increase in density of the negative charge in the rgion where they overlap. This creates an increase in negative charge between the nuclei and an-increase in the plus-minus attraction between the electron and the nuclei for the atoms in the bond.

The greater attraction leads to lower potent energy because electrons in the molecular orbital are lower potential energy than in separate atomic orbitals energy would be required to shift the electrons back into **(1s)** orbitals, of separate atoms. This keeps the atoms together in the molecule. So we call this orbital a bonding molecular orbital.

The second way that atomic orbitals interact is (out-of phase). Where the atomic orbitals overlap the out-of-phase interaction leads to a decrease in the intensity of the negative charge this creates a decrease in negative charge between the nuclei and decrease in plus-minus attraction between electron charge and the nuclei of the atoms in the bond. The lesser attraction leads to higher potential energy. The electrons are more stable in the is atomic orbitals of separate atoms so electrons in this type of molecular orbital destabilize the bond between atoms we call molecular orbitals of this type (anti bonding molecular orbitals).

First have the **1s + 1s** $\longrightarrow$ σ (sigma) bonding MO and then above this σ^*(sigma star) antibonding MO.

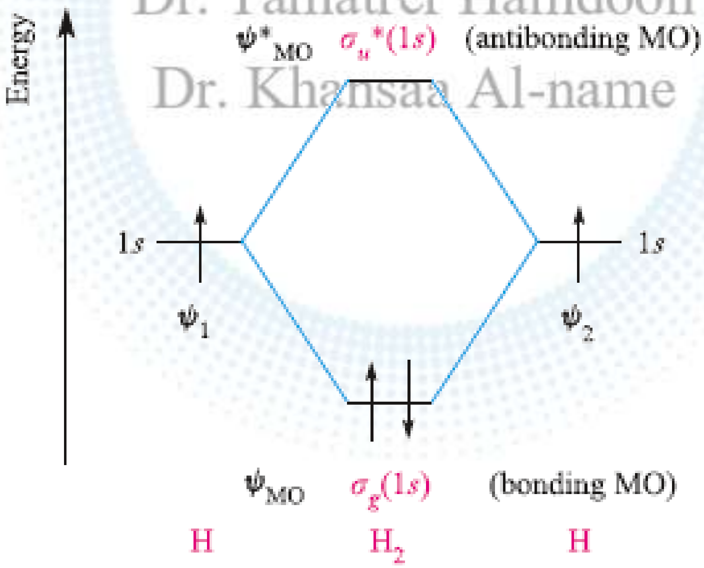


Fig. 2.4 An orbital interaction diagram for the formation of H_2 from two hydrogen atoms. By the *aufbau* principle, the two electrons occupy the lowest energy (bonding) molecular orbital.

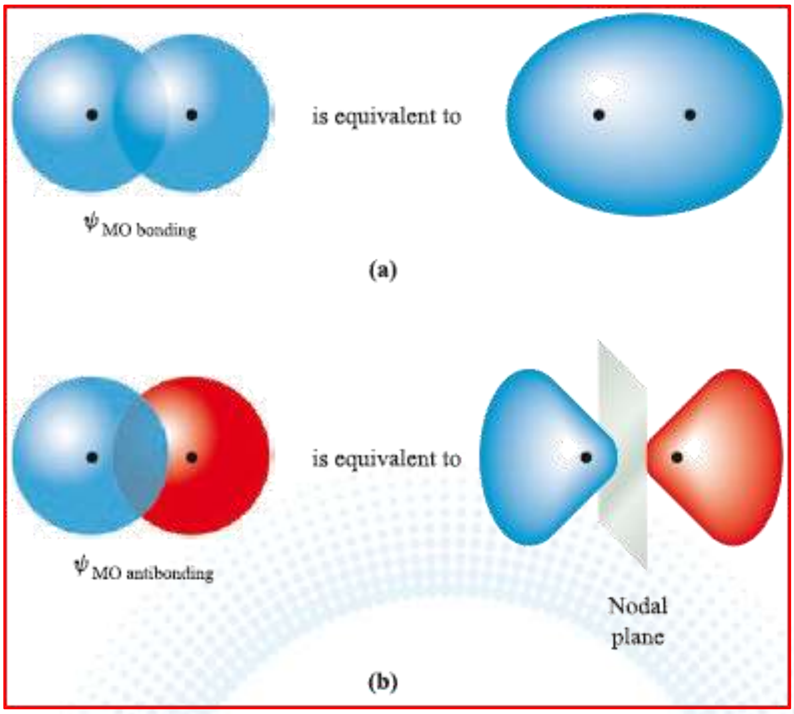


Fig 2.5:The symetry of sigma MO (a) and sigma star MO(b)

Then; there are the pair 2s + 2s bonding σ and anti bonding σ^*

Next, we come to **p** and **p** interactions, the **2p$_x$ + 2p$_x$** orbital interaction give **σ 2p$_x$**, the **2p$_y$ + 2p$_y$** and **2p$_z$ + 2p$_z$** interaction are equivalent, they only differ in spatial orientation, Both give rise to π bonding and π^* anti bonding. This gives a ground state electronic configuration of:

$\sigma 1s^2 \quad \overset{*}{\sigma} 1s^2 \quad \sigma 2s^2 \quad \overset{*}{\sigma} 2s^2 \quad (\pi 2p^2_y \equiv \pi 2p^2_z)\ \sigma 2p^2_x$

$(\overset{*}{\pi} 2p^2_y \equiv \overset{*}{\pi} 2p^2_z)\ \overset{*}{\sigma} 2p^2_x$

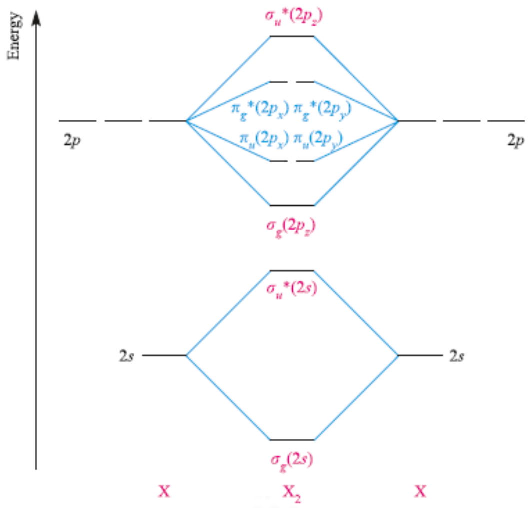


Fig. 2.8 A general orbital interaction diagram for the formation of X_2 in which the valence orbitals of atom X are the 2s and 2p. In constructing this diagram we assume that the s–p separation is sufficiently large that no orbital mixing occurs. The X nuclei lie on the z axis.

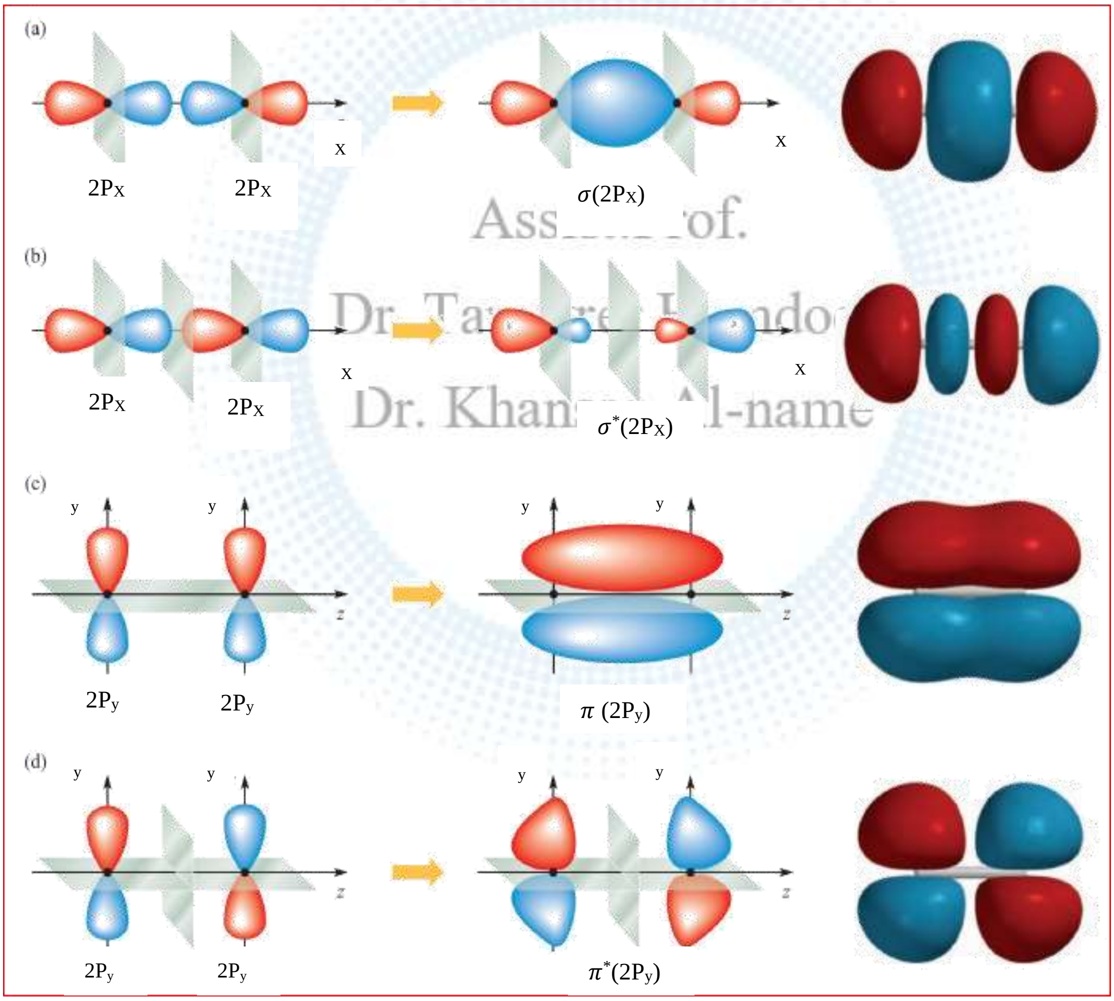


Fig. 2.7 The overlap of two 2p atomic orbitals for which the atomic nuclei are defined to lie on the z axis: (a) direct overlap along the z axis gives a $\sigma_g(2p_z)$ MO (bonding); (b) the formation of the $\sigma_u^*(2p_z)$ MO (antibonding); (c) sideways overlap of two $2p_x$ atomic orbitals gives a $\pi_u(2p_x)$ MO (bonding); (d) the formation of $\pi_g^*(2p_x)$ MO (antibonding). Atomic nuclei are marked in black and nodal planes in grey. The diagrams on the right-hand side are more realistic representations of the MOs and have been generated computationally using Spartan '04, ©Wavefunction Inc. 2003.

Homo nuclear diatomic Molecules:

1- Dihydrogen: H_2

$$\left.\begin{array}{l} H \quad 1s^1 \\ H \quad 1s^1 \end{array}\right] \xrightarrow{2e} \sigma_{1S}^2$$

$\sigma 1_S$ (HOMO) Highest Occupied Molecular Orbital.

$\sigma^* 1_S$ (LUMO) Lowest Unoccupied Molecular Orbital.

bond order: is defined as the number of electrons in bonding **MO** minus the number of electrons in antibonding **MO** divided by two.

$$\textbf{bond order} = \frac{\text{number of es.in bonding MO} - \text{number of es in an antibonding MO}}{2}$$

for $H_2 = \frac{2-0}{2} = 1$

H —— H

Because there are no unpaired electrons it is diamagnetic and stable molecule, type of bond is (**σ** bond)

Ex: Use the diagram of **MO** to determine the bond order, then describe the bonding and the magnetic properties for the following:

He_2, Li_2, Be_2, B_2, C_2, N_2, F_2, Ne_2

Dihelium **He_2**

$$\left.\begin{array}{l} {}_2He \quad 1s^2 \\ {}_2He \quad 1s^2 \end{array}\right] \xrightarrow{4e^-} \sigma_{1S}^2 \quad \sigma^*_{1S}{}^2$$

bond order $= \frac{2-2}{2} = 0$

∴ unknown molecule (it is unstable), if He_2 did form, it would be diamagnetic

Dilithium **Li_2**

$$\left.\begin{array}{l} {}_3\mathrm{Li}\ 1s^2\ \ 2s^1 \\ {}_3\mathrm{Li}\ 1s^2\ \ 2s^1 \end{array}\right] \xrightarrow{6e^-} \sigma_{1s}{}^2\ \ \ \sigma^*{}_{1s}{}^2\ \ \ \sigma_{2s}{}^2$$

bond order= $\frac{4-2}{2}$

bond order = **1** ∴ (**σ** bond**)**

it is diamagnetic, it is stable (known in the gase phase)

Diberyllium **Be_2**

$$\left.\begin{array}{l} {}_4\mathrm{Be}\ \ 1s^2\ \ 2s^2 \\ {}_4\mathrm{Be}\ \ 1s^2\ \ 2s^2 \end{array}\right] \xrightarrow{8e^-} \sigma 1s^2\ \ \ \sigma^* 1s^2\ \ \ \sigma 2s^2\ \ \sigma^* 2s^2$$

bond order= $\frac{4-4}{2}$

bond order = zero It is unknown

Diboron**: B_2**

$$B_2 = 10e^-:\ \sigma 1s^2\ \ \overset{*}{\sigma} 1s^2\ \ \ \sigma 2s^2\ \overset{*}{\sigma} 2s^2\ (\pi 2p^1{}_y \equiv \pi 2p^1{}_z)$$

Bond order = $\frac{6-4}{2} = 1$

It is known in the gas phase (diradical) and paramagnetic

Dicarbon **C_2**

$$C_2 = 12e^- = \sigma 1s^2\ \ \ \sigma^* 1s^2\ \ \ \sigma 2s^2\ \overset{*}{\sigma} 2s^2\ (\pi 2p^2{}_y \equiv \pi 2p^2{}_z)$$

bond order = $\frac{8-4}{2} = 2$

∴ 1 σ; 1π bonds

It is know in the gase phase diamagnetic **:C = C:**

$$N_2 = 14e- = \sigma 1s^2\ \ \ \sigma^* 1s^2\ \ \ \sigma 2s^2\ \ \sigma^* 2s^2\ (\pi_2 p^2{}_y \equiv \pi_2 p^2{}_z)\ \sigma_2 p^2{}_x$$

bond order = $\frac{10-4}{2} = 3$ **:N ≡ N:**

∴ 1 σ, 2π It is diamagnetic

Oxygen: O_2 **=16 e**$^-$

$\sigma 1s^2 \quad \sigma^* 1s^2 \quad \sigma 2s^2 \ \sigma^* 2s^2 \ \sigma 2p^2_x \ (\pi 2p^2_y \equiv \pi 2p^2_z) \ (\pi 2p^1_y \equiv \pi 2p^1_z)$

bond order = $\frac{10-6}{2}$

bond order $= 2 \quad \therefore 1\ \sigma, 1\pi \qquad :\dot{O}=\dot{O}:$

paramagnetic; diradical

$O_2 \ \ t = 2 \times 8 = 16 \qquad v = 2 \times 6 = 12$

$b = \frac{t-v}{2} \qquad n.\ b = \frac{v-2b}{2}$

$b = \frac{16-12}{2} = 2 \qquad n.b = \frac{12-4}{2} = 4$ **peris** $\qquad :\ddot{O}=\ddot{O}:$

Diflourine: F_2

$F_2 = 18e^-$

$\sigma 1s^2 \quad \sigma^* 1s^2 \quad \sigma 2s^2 \ \sigma^* 2s^2 \ \sigma 2p^2 x \ (\pi 2p^2_y \equiv \pi 2p^2_z) \ (\pi^* 2p^2_y \equiv \pi^* 2p^2_z) \ \sigma^* 2p_x$

bond order= $\frac{10-8}{2}$

bond order $= 1$ stable and diamagnetic $\qquad :\underset{..}{\ddot{F}} - \underset{..}{\ddot{F}}:$

Dineon: Ne_2

$Ne_2 = 20e^-$

$\sigma 1s^2 \quad \sigma^* 1s^2 \quad \sigma 2s^2 \ \sigma^* 2s^2 \ \sigma 2p^2_x \ (\pi 2p^2_y \equiv \pi 2p^2_z) \ (\pi^* 2p^2_y \equiv \pi^* 2p^2_z) \ \sigma^* 2p^2_x$

bond order= $\frac{10-10}{2}$ = zero

The bond order suggests that Ne_2 is unstable if Ne_2 did form it would be diamagnetic.

We describe the stability of molecule with bond order.

If the bond order = zero the molecule is unstable and unknown.

If the bond order greater than zero the molecule is stable.

The higher bond order is the more stable bond.

Q1/ Rank the following molecules according to increase in stability, And show why?

$\mathbf{Ne_2}$, $\mathbf{O_2}$, $\mathbf{F_2}$, $\mathbf{N_2}$

Q2/ using the (MO) diagram to rank the following ions and molecule according of decrease in the bond distance?

$\mathbf{N_2}$, $\mathbf{N_2^-}$, $\mathbf{N_2^+}$

$N_2 = 14e^-$: $\sigma 1s^2 \quad \overset{*}{\sigma} 1s^2 \quad \sigma 2s^2\ \overset{*}{\sigma} 2s^2\ (\pi 2p^2_y \equiv \pi 2p^2_z)\ \sigma 2p^2_x$

Bond order= $\frac{10-4}{2} = 3$ $\quad \ddot{N} \equiv \ddot{N}$

$N_2^- = 15e^- = \sigma 1s^2 \quad \overset{*}{\sigma} 1s^2 \quad \sigma 2s^2\ \overset{*}{\sigma} 2s^2 \quad \sigma 2p^2_x\ (\pi 2p^2_y \equiv \pi 2p^2_z)\ (\overset{*}{\pi} 2p^1_y \equiv \overset{*}{\pi} 2pz)$

bond order = $\frac{10-5}{2} = 2.5$ $\quad (:\underline{N} = \dot{N}:)^-$

$N_2^+ = 13\ e^+ = \sigma 1s^2 \quad \overset{*}{\sigma} 1s^2 \quad \sigma 2s^2\ \overset{*}{\sigma} 2s^2\ (\pi 2p^2_y \equiv \pi 2p^2_z)\ \sigma 2p^1_x$

bond order = $\frac{9-4}{2} = 2.5$ $\quad (:\underline{N} = \dot{N}:)^+$

$N_2 < N_2^- = N_2^+$

Isoelectronic Species:

Species are isoelectronic if they have the same total number of electrons.

Ex: $[BH_4]^-$, CH_4 and **$[NH_4]^+$** are isoelectronic

$[BH_4]^- = 10e^-$, $CH_4 = 10e^-$, $[NH_4]^+ = 10e^-$

Q/ show that **$[N_2]$** and **$[NO]^+$** are isoelectronic.

Q/ Using the **MO** diagram to show that **$[CN]^-$** and **$[NO]^+$** are isoelectronic

Electronegativity: χ

Is a character of atom when combined with other atoms (not for separated atoms).

Electronegativity: is the measurement of an atom to compete for the electrons in a bond. The higher Electronegativity, the greater it's ability to gain electrons in a bond. Electronegativity will be important when we later determine polar and nonpolar molecules.

In homonuclear diatomic molecules **A_2**, the electron density in the region between the nuclei is symmetrical, each atom **(A)** possess same $\overset{*}{Z}$.

In heteronuclear diatomic molecules AB, the electron density in the region between the two nuclei is asymmetric, each atom **(A, B) if $\overset{*}{Z}B > \overset{*}{Z}A$** the pair of electrons will be drawn toward **B** and away form **A**

A —— A , $A^{+\delta}$ —— $B^{-\delta}$, A^+ B^-
Pure covalent polar covalent ionic

Pauling electronegativity values χ^P

in the early **1930** Linus Pauling established the concept of electronegativity which he defined as (the power of an atom in a molecule to attract electrons to itself) the electron with drawing power of an atom.

Electronegativity and bond Dissociation Energy:

$D(A-B)_{cal} = {}^{1}/_{2}\,[D(A-A) + \quad D(B-B)]$

$D(A-B)$ experimental $> D(A-B)_{cal}$

$D(A-B)_{exp} = D(A-B)_{cal} + \Delta D$

$\Delta D = D(A-B)_{exp} - D(A-B)_{cal}$

$\Delta\chi = \sqrt{\Delta D_{AB}} = \chi^{P}(A) - \chi^{P}(B)$……………………………………...….(1)

ΔD = Ionic resonance energy units of $\Delta D = eV$

Ex/ Using the following data to estimate a value for **D (Br – F)**:

$D(F-F) = 158$ K.J/mol , $D(Br-Br) = 224$ K.J/mol

$\chi^{P}(F) = 4.0eV$; $\chi^{P}(Br) = 3.0eV$

$\sqrt{\Delta D} = \chi^{P}(F) - \chi^{P}(B) = 4-3 = 1.0\ eV$

$\therefore \Delta D = 1^{2} = 1$

This gives the value in **eV**; convert to **KJ/mol**

1.0 ev = 96.5 KJ/mol

$\therefore \Delta D = 1\ eV = 96.5$ KJ/mol

$D(Br-F)_{cal} = {}^{1}/_{2}\,[D(F\text{-}F) + D(Br-Br)]$

$= \frac{158+224}{2} = \frac{382}{2} = 191$ KJ/mol

$D_{exp} = D_{cal} + \Delta D$

$D(Br\text{-}F)_{exp} = D(Br-F)_{cal} + \Delta D$

$= 191 + 96.5 = 287.5$ KJ/mol

H.W/ use the following data to estimate the bond dissociation enthalpy of BrCl:

D (Br – Br) = 224 K.J/mol ; D (Cl – Cl) = 242 K.J/mol

χ^P (Br) = 3.0 ev **χ^P (Cl) = 3.2 ev**

Electronegativity Scales:

1- Pauling's Bond Energy scale (1930) χ^P :

Pauling's method makes a use of bond dissociation as shown above equation **(1)** gives electronegativity difference values. This equation can be used to calculate χ value of an atom provided that χ value of the other element is known. Pauling assigned an arbitrary value of **4.0** for the electronegativity of fluorine and calculated that of other elements with the help of this equation.

Table: Electronegativity values of s- and p- block elements as determined by Pauling (scale F = 4.0)

s-block elements		p-block elements				
I A 1	**II A 2**	**III A 13**	**IV A 14**	**V A 15**	**VI A 16**	**VII A 17**
H 2.1						
Li 1.0	Be 1.5	B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Na 0.9	Mg 1.2	Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0
K 0.8	Ca 1.0	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8
Rb 0.8	Sr 1.0	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5
Cs 0.7	Ba 0.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2	At 2.2
Fr 0.7	Ra 0.9					

Electronegativity also affected by the bond order it increase as bond order increase.

C – C , C = C , C ≡ C
χ^P = 2.5 , 2.75 , 3.3

2- Mullikan Electronegativity scale **(1934) χ^M**

χ^M is the average of **$I.P_1 + E.A_1$**

$$\chi^M = \frac{I.P_1 + E.A_1}{2} \text{ in e.V}$$

Disadvantage

1- The values of **EA_1** are not readily available.

2- The quantities **$I.P_1$** and **EA_1** refer to the equivalent state of the atom in a molecule (number of electronic states that could be achieved by the atom in a molecule), since the equivalent state of an atom is different as the molecule different, so χ^M for atom will be different.

3- Allred Rochow Electronegativity scale χ^{AR} **(1958)**.

depends on **Z^*** and **r_{cov}** (in **pm**)

$$\chi^{AR} \propto \frac{Z^*}{r2_{cov}}$$

$$\chi^{AR} = (3590\frac{Z^*}{r2_{cov}} + 0.744)$$

All three scales are of similar trend. The most electronegative elements are

F , O , Cl $\chi > 1$

The most electro positive elements are

Li , Na , Cs $\chi < 1$

Trend in Electronegative

1- χ increases from left to right in a period (because $\overset{*}{Z}$ increases). As we add additional electrons on crossing a period, we are also adding additional protons, which are only **0.35** shielded by the additional electrons hence all valance electrons (including those in the bond) are more strongly attracted to the nucleous.

2- Down group 1 and 2 , $\overset{*}{Z}$ often remain constant so the small decline in the electronegativity is due to the larger size.

3- Elements with high ionization energies have high electronegativities due to (the strong pull exerted by the positive nucleus on the negative electrons. Therefore the electronegativity in creases from bottom to top and from left to right

MOT for Hetero nuclear diatomic molecules

e.g/ HF hydrogen fluoride

$_1$**H: 1s**^{1} : $_9$**F** : **1s**^{2} **2s**^{2} **2p**^{5}

$\overset{*}{Z}$ of **(F)** > $\overset{*}{Z}$ of **(H)**

∴ χ of (F) > χ of **(H)**

Overlap between the **1s** of H and **2s** of F is allowed by symmetry, but the energy separation is very large, Overlap between **H 1s** and **F 2p$_x$** symmetry allowed and there is reasonable orbital energy match.

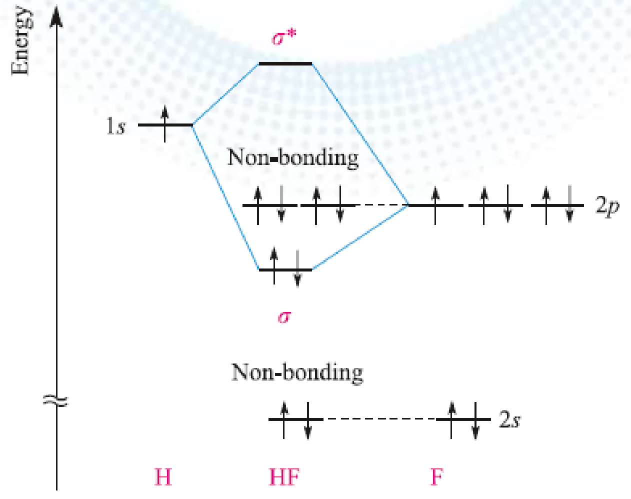


Fig: 2-8 An orbital interaction diagram for the formation of HF. Only the valence atomic orbitals and electrons are shown. The break in the vertical (energy) axis indicates that the energy of the F 2*s* atomic orbital is much lower than is actually shown.

CO carbon monoxide:

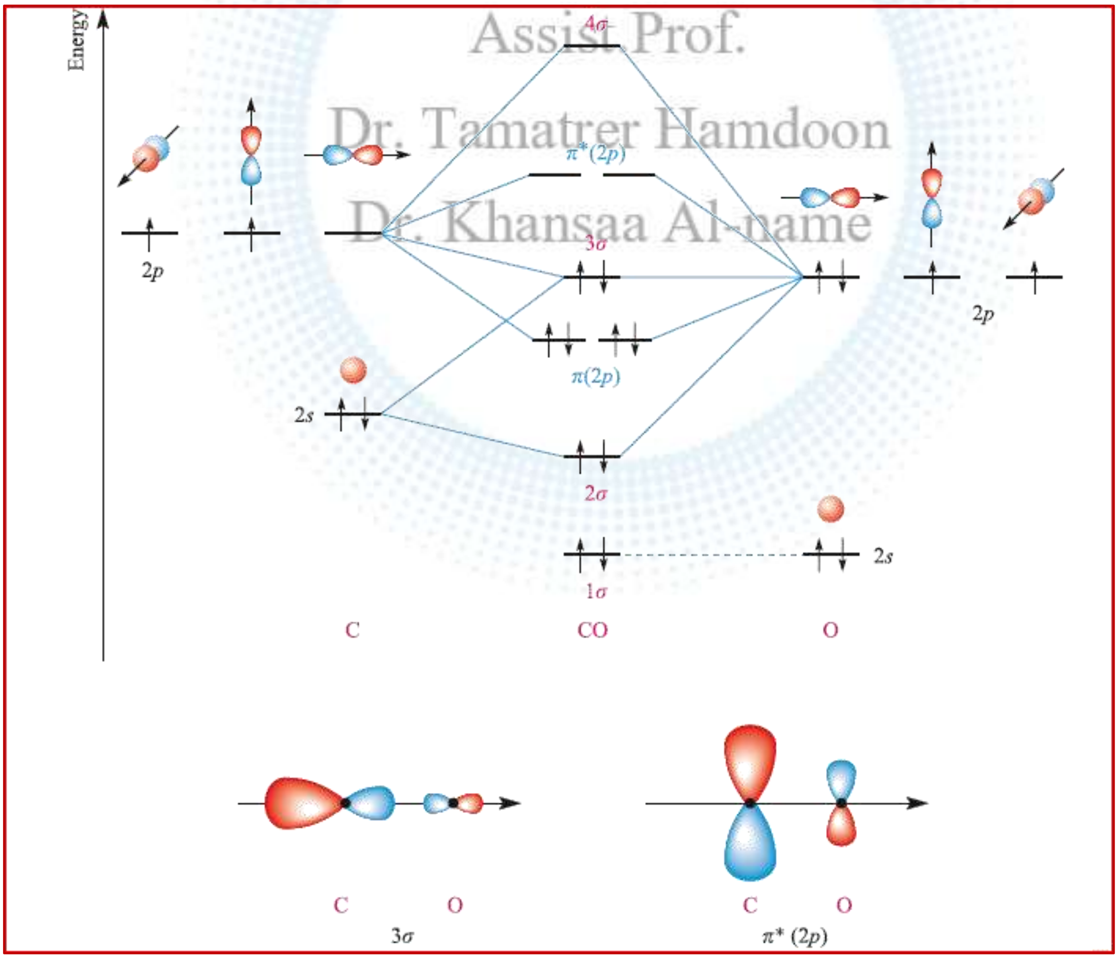
We must take note of the following

- **$\overset{*}{Z}$ (O) > $\overset{*}{Z}$ (C)**
- The energy of the **O 2s** atomic orbital is lower than that of **C 2s** atomic orbital.
- The **2p** level in **O** is at lower energy than that of **C**.
- The **2s – 2p** energy separation in **O** is greater than that in **C**.

$_6C + _8O = 14e^-$

$\sigma 1s^2$ $\overset{*}{\sigma}1s2$ $\sigma 2s^2$ $\sigma\overset{*}{2}s^2$ $(\pi 2p^2_y \equiv \pi 2p^2_z)$ $\sigma 2p^2_x$

Bond order= $\frac{10-4}{2}$= 3



Q/ Use the **MOT** diagram to rank the following oxygen species

$[O_2]^+$, $[O_2]^-$, $[O_2]^{-2}$, O_2

according to increase of (Bond distance), which of these species are paramagnetic.

Q/ Lewis structure show that **O_2** is diamagnetic is the **MOT** consistent with this fact**?**

Q/ a) Why **Na_2O_2** described as colourless while **NaO_2** is colour

b) Na_2O_2 is diamagnetic while **NaO_2** is paramagnetic**?**

$Na_2^{+2}\,[O_2]^{-2}$ ⇒ contain **$[O_2]^{-2}$** peroxide

$[O_2]^{-2} = 16e + 2e = 18e$

$\sigma 1s^2 \quad \overset{*}{\sigma}1s^2 \quad \sigma 2s^2 \quad \overset{*}{\sigma}2s^2 \quad \sigma 2p^2_x \quad (\pi 2p^2_y = \pi 2p^2_z)\ (\overset{*}{\pi}2p^2_y = \overset{*}{\pi}2p^2_z)$

Bond order= $\frac{10-8}{2} = 1$

There is no unpaired electron so it is colorless and diamagnetic

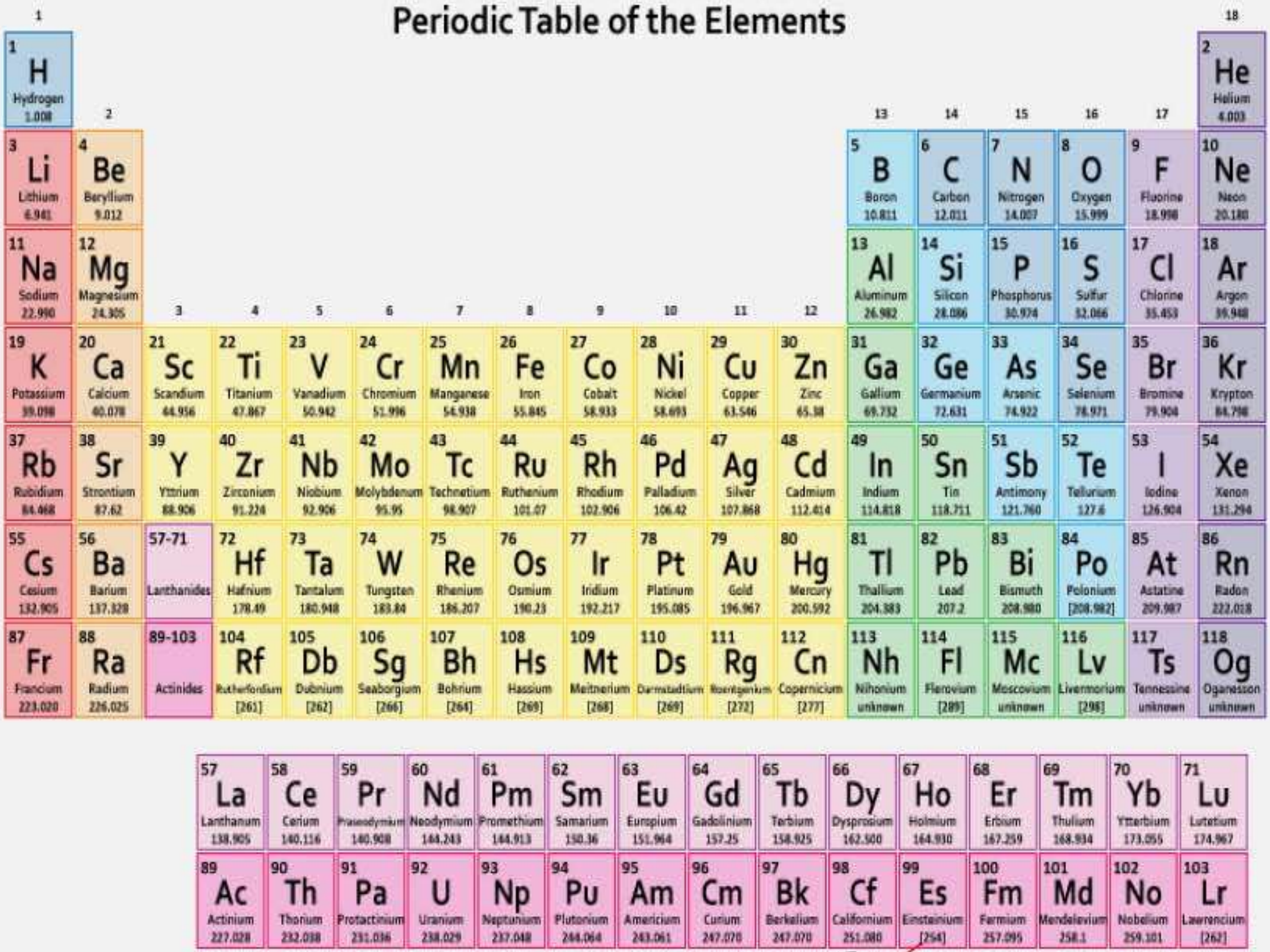
NaO_2 ⇒ contain **$[O_2]^{-1}$** superoxides

$[O_2]^{-1} = 16e^- + 1e^- = 17e^-$

$\sigma 1s^2 \quad \overset{*}{\sigma}1s^2 \quad \sigma 2s^2 \quad \overset{*}{\sigma}2s^2 \quad \sigma 2p^2_x \quad (\pi 2p^2_y = \pi 2p^2_z)\ (\overset{*}{\pi}2p^2_y = \overset{*}{\pi}2p^1_z)$

Bond order= $\frac{10-7}{2} = 1.5$

There is an unpaired electron so it is colour and paramagnetic.



Periodic Table of the Elements

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 H Hydrogen 1.008																	2 He Helium 4.003
3 Li Lithium 6.941	4 Be Beryllium 9.012											5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180
11 Na Sodium 22.990	12 Mg Magnesium 24.305											13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.066	17 Cl Chlorine 35.453	18 Ar Argon 39.948
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.867	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.732	32 Ge Germanium 72.631	33 As Arsenic 74.922	34 Se Selenium 78.971	35 Br Bromine 79.904	36 Kr Krypton 84.798
37 Rb Rubidium 84.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.95	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.414	49 In Indium 114.818	50 Sn Tin 118.711	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904	54 Xe Xenon 131.294
55 Cs Cesium 132.905	56 Ba Barium 137.328	57-71 Lanthanides	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.217	78 Pt Platinum 195.085	79 Au Gold 196.967	80 Hg Mercury 200.592	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [208.982]	85 At Astatine 209.987	86 Rn Radon 222.018
87 Fr Francium 223.020	88 Ra Radium 226.025	89-103 Actinides	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [268]	110 Ds Darmstadtium [269]	111 Rg Roentgenium [272]	112 Cn Copernicium [277]	113 Nh Nihonium unknown	114 Fl Flerovium [289]	115 Mc Moscovium unknown	116 Lv Livermorium [298]	117 Ts Tennessine unknown	118 Og Oganesson unknown

57 La Lanthanum 138.905	58 Ce Cerium 140.116	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.243	61 Pm Promethium 144.913	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.500	67 Ho Holmium 164.930	68 Er Erbium 167.259	69 Tm Thulium 168.934	70 Yb Ytterbium 173.055	71 Lu Lutetium 174.967
89 Ac Actinium 227.028	90 Th Thorium 232.038	91 Pa Protactinium 231.036	92 U Uranium 238.029	93 Np Neptunium 237.048	94 Pu Plutonium 244.064	95 Am Americium 243.061	96 Cm Curium 247.070	97 Bk Berkelium 247.070	98 Cf Californium 251.080	99 Es Einsteinium [254]	100 Fm Fermium 257.095	101 Md Mendelevium 258.1	102 No Nobelium 259.101	103 Lr Lawrencium [262]

Alkali Metal	Alkaline Earth	Transition Metal	Basic Metal	Semimetal	Nonmetal	Halogen	Noble Gas	Lanthanide	Actinide