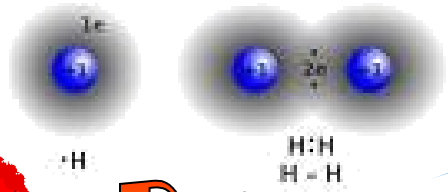
A

Chemical Bonding & Molecular Structure

Chemical Bonding & Molecular Structure

CHEMISTRY PROJECT WORK



By-

Akarshik Banerjee

Pratyush Dey

Sayantan Biswas

Class- XI 'B'

P

Matter is made up of on or different elements. But under normal conditions except noble gasses no other elements occur as single atom. Evidently there is a force which holds together various constituent particles in different chemical species.

This force is called the-

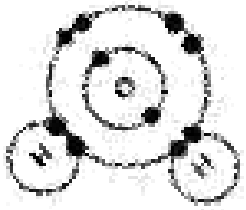
Chemical Bond

s

KOSSEL - LEWIS APPROACH TO CHEMICAL BONDING

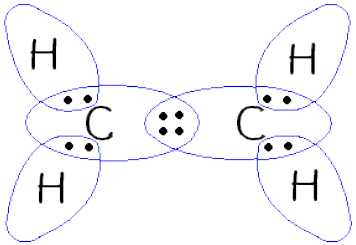
Octet Rule

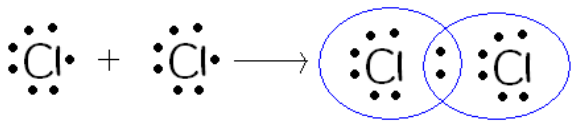
As per electronic theory of chemical bonding atoms combine to attain noble gas configuration.



Covalent Bond

When two or more atoms share electron pairs they are said to be covalently bonded.

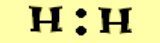
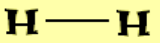
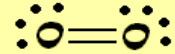
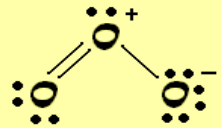
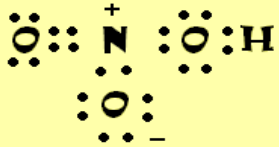
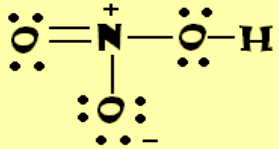




Lewis Structures

Lewis dot structures provide a picture of bonding in molecules and ions in terms of shared pairs of electrons and octet rule.

A few examples are–

Molecule / ion		Lewis representation
H_2		
O_2		
O_3		
HNO_3		

P

Formal Charge

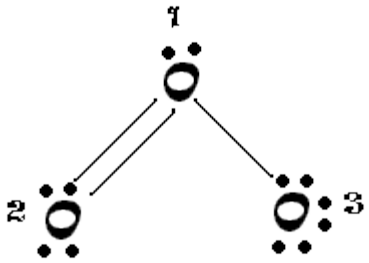
Formal charge(F.C) on an atom in a Lewis structure =

$$\left[\text{Total no. of valence electrons in free atom}\right] - \left[\text{Total no. of lone pairs electrons}\right] - (1/2)\left[\text{Total no. of bonding electrons}\right]$$

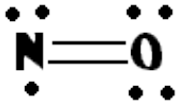
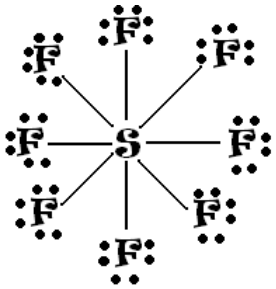
Ex-

Formal charge on each O atom are:-

- *On O no.1= 6 - ½ - ½ (6)=1*
- *On O no. 2= 6 - 4 - ½ (2)=0*
- *On O no.3= 6 - 6 - ½ (2)= - 1*

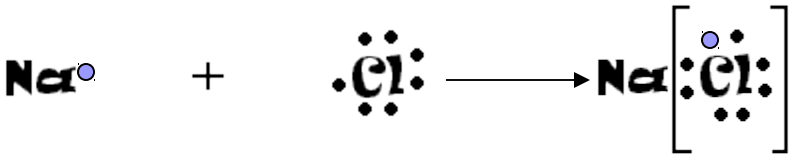


Limitations of Octet Rule

- The incomplete octet of central atom. → 
- Odd electron molecules. → 
- The expanded Octet. → 

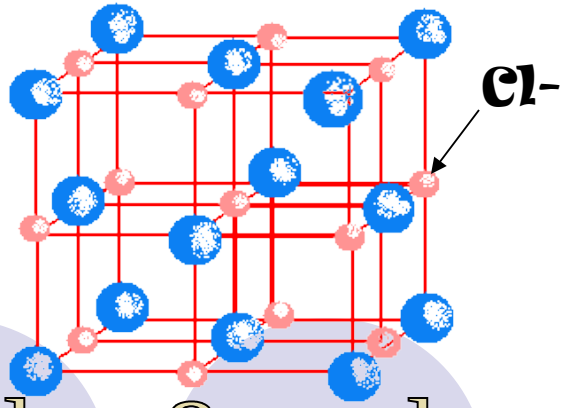
Electrovalent Bond

When two or more elements form a bond by complete transfer of electrons the bond is said to be electrovalent bond.



A

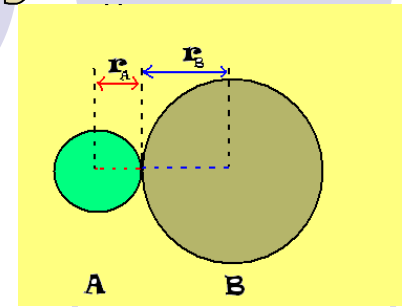
Lattice Enthalpy



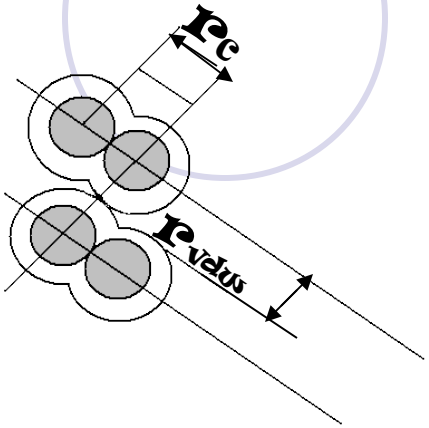
It is defined as the energy required to completely separate one mole of solid ionic compound to gaseous constituent ions.

Bond length, Angle, Enthalpy& order

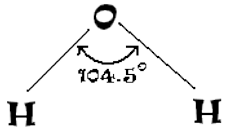
- **Covalent radius** *is measured as the radius of an atom's core which is in contact with the core of adjacent atom in bonded situation.*



- **Van der Waals** *radius represents the overall size of the atom which includes its valence shell in non -bonded situation.*



- **Bond angle** *is the angle between the orbitals containing the electron pairs around the central atom/molecule/ complex ion.*



- **Bond enthalpy** *is the energy required to break one mole of like bonds in two atoms in gaseous state.*

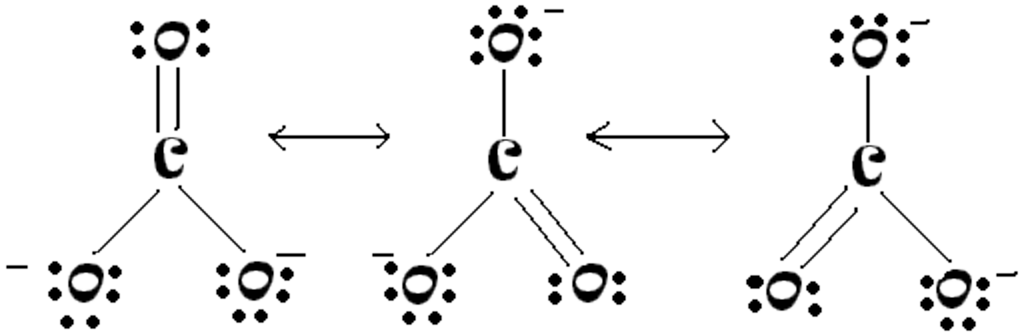
- **Bond order** *is the no. of bonds between two elements in a molecule.*

P

Resonance Structures

Whenever a single Lewis structure cannot describe a molecule accurately, a no. of structures with similar energy, positions of nuclei, bonding & non bonding pairs of electrons are taken as the canonical structure of the hybrid which describes the molecule accurately.

Resonance in CO_3^{-2} represent the three canonical forms:-

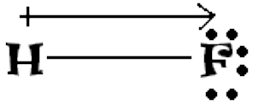


s

Polarity of Bonds

In heterogeneous covalent compounds due to greater electronegativity of one atom the shared electron pair ins displaced more towards it than the other molecule.

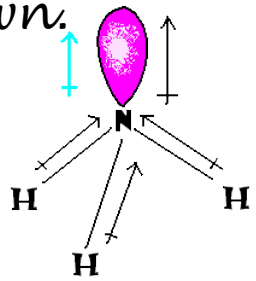
As a result of polarization the molecule posses a net **Dipole moment** (depicted as a small arrow with the tail in the positive center and head on the negative center.)

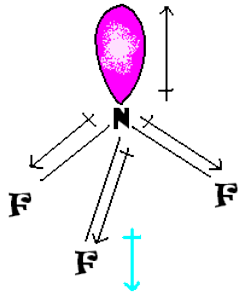


Dipole moment = charge **x** distance of separation

By knowing the dipole moment the symmetry or the polarity of a molecule can be known.

The net Dipole moment of NF_3 is less than NH_3 despite fluorine being more electronegative is due to the fact that the arrows are in opposite directions in both cases and the lone pair adds to the dipole moment in the latter but decreases the dipole moment in the former.





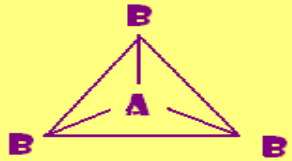
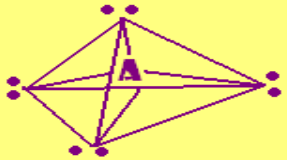
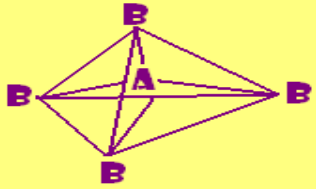
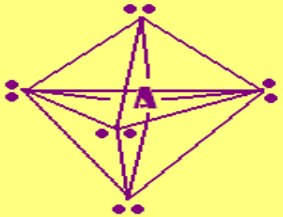
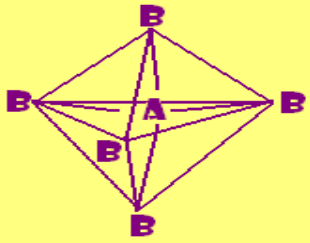
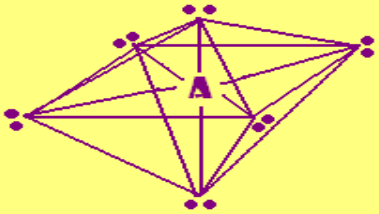
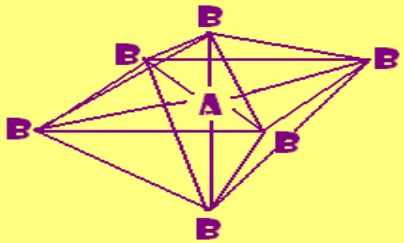
P

Valence Shell Electron Pair Repulsion Theory

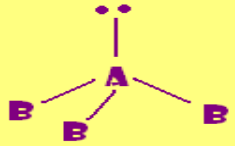
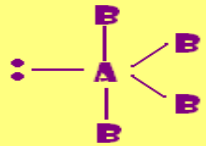
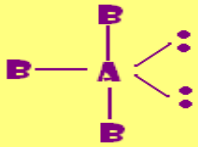
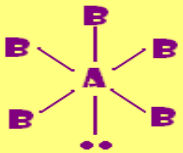
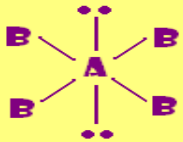
- The shape of a molecule depends upon the no. of valence electrons.
- Pairs of electrons repel each other.
- They tend to occupy such positions so as to minimise repulsion and maximise distance between them.
- The valance shell is taken as a sphere .
- A multiple bond is treated as a single electron pair and single electron pairs in multiple bonds are treated as a single super pair.
- The VESPER model is applicable to any such structure where two or more resonance structures can represent a molecule.

VSEPR Theory is able to predict the geometry of large no. of molecules especially the compounds of p-block elements accurately.

Geometry of molecules in which central atom has no lone pairs

ELECTRON PAIRS	ARRANGEMENT OF ELECTRON PAIRS	MOLECULAR GEOMETRY	EXAMPLES
2		 LINEAR	$BeCl_2$
3		 TRIAGONAL PLANAR	BF_3
4		 TETRAHEDRAL	Ch_4
5		 TRIAGONAL BIPYRAMIDAL	PCl_5
6		 OCTAHEDRAL	SF_6

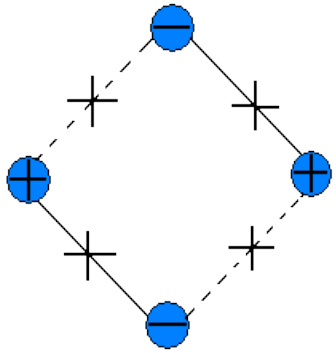
Geometry of molecules in which central atom has 1 Or more lone pairs

MOLECULAR TYPE	NO. OF BOND PAIRS	NO. OF LONE PAIRS	ARRANGEMENT OF ELECTRON PAIRS	SHAPE	EXAMPLES
AB_2E	2	1		BENT	SO_2
AB_3E	3	1		TRIAGONAL PYRAMIDAL	NH_3
AB_2E_2	2	2		BENT	H_2O
AB_4E	4	1		SEE SAW	SF_4
AB_3E_2	3	2		T- SHAPE	ClF_3
AB_5E	5	1		SQUARE PYRAMID	BrF_5
AB_4E_2	4	2		SQUARE PLANAR	XeF_4

s

VALANCE BOND THEORY

As two atoms approach each other the following forces come into action:-

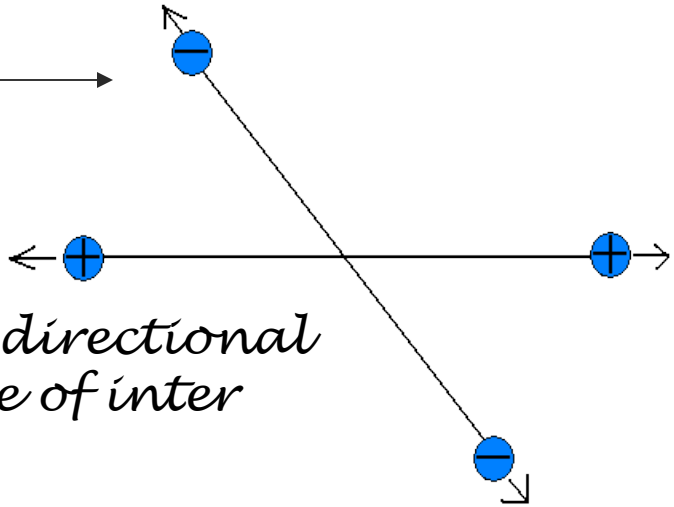


Attractive forces between-

a) Nucleus of an atom & its own electrons.

b) Nucleus of one atom & electrons of the other atom.

Repulsive forces between-



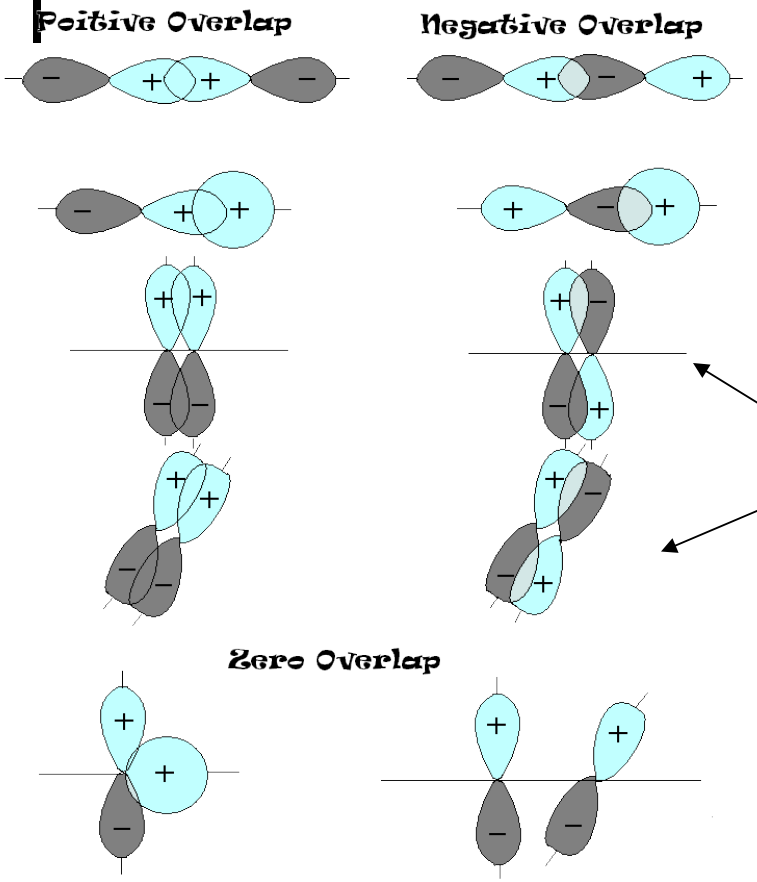
a) Electrons of two atoms.

b) Nuclei of two atoms.

The valance bond theory explains the directional properties of bond as a consequence of inter electronic repulsion.

A

Types of overlapping

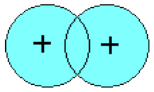


p-p overlapping (sigma Bond)

s-p overlapping (sigma Bond)

p-p overlapping (pi Bond)

s-s overlapping (sigma Bond)



Strengths – *The strengths of bonds depends upon the extent of overlap. So sigma bond has more strength than pi bond.*

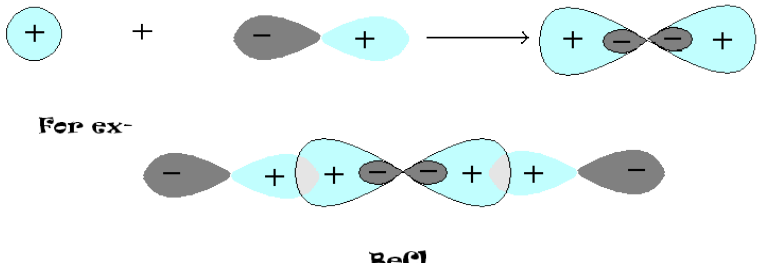
A

HYBRIDISATION

Hybridisation is the process of intermixing of the orbitals of slightly different energies in order to redistribute their energies to form new set of orbitals with equivalent energy and shape.

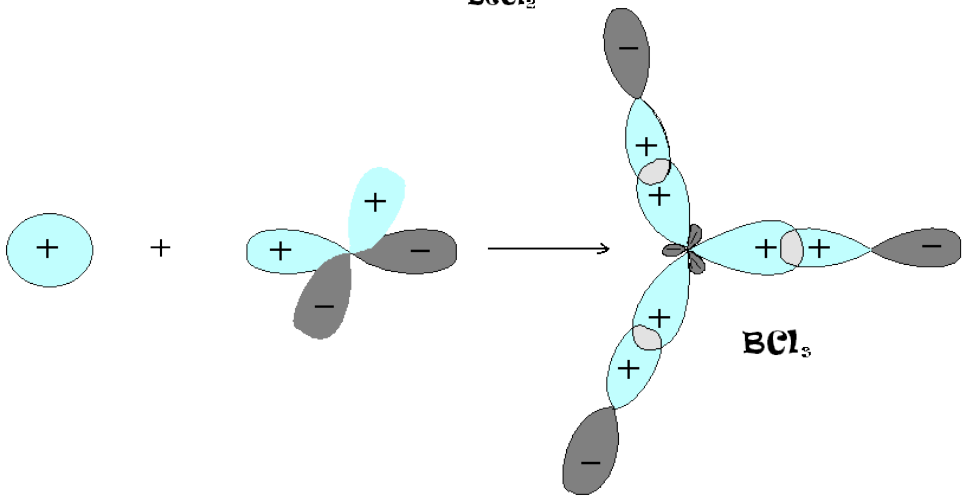
S-p hybridisation

It involves mixing of 1S orbital and 1p orbital



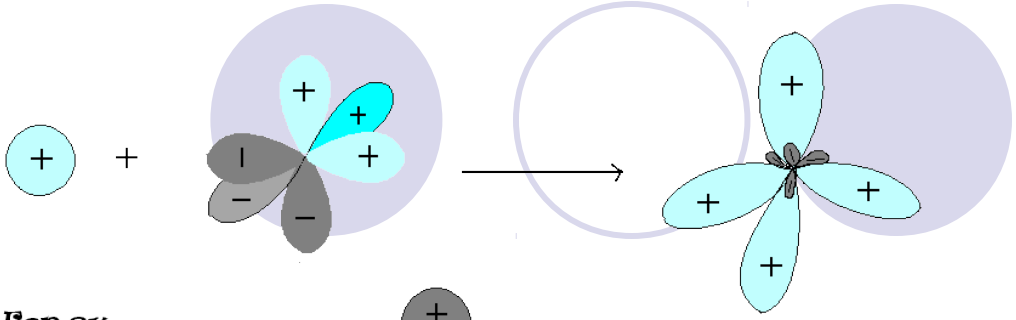
S-p^2 hybridisation

It involves mixing of 1S and 2p orbitals.



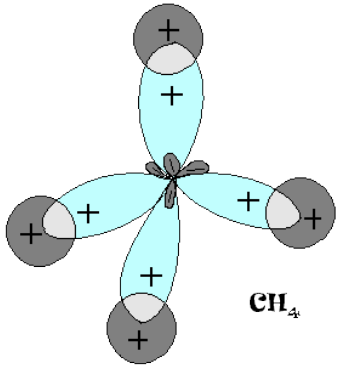
A

$S-p^3$ hybridisation



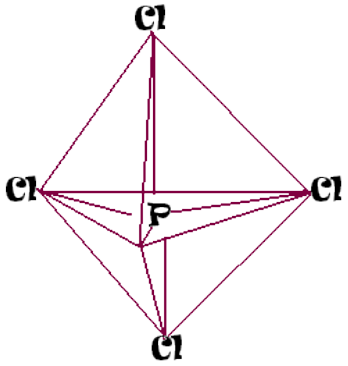
It involves mixing of 1S and 3p orbitals.

For ex-

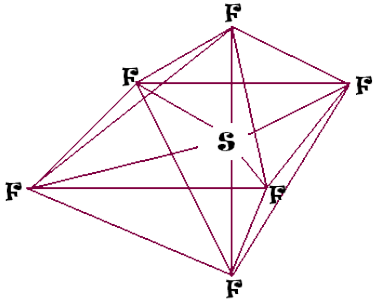


Hybridisation involving d orbitals

$S-p^3d$ hybridisation



$S-p^3d^2$ hybridisation



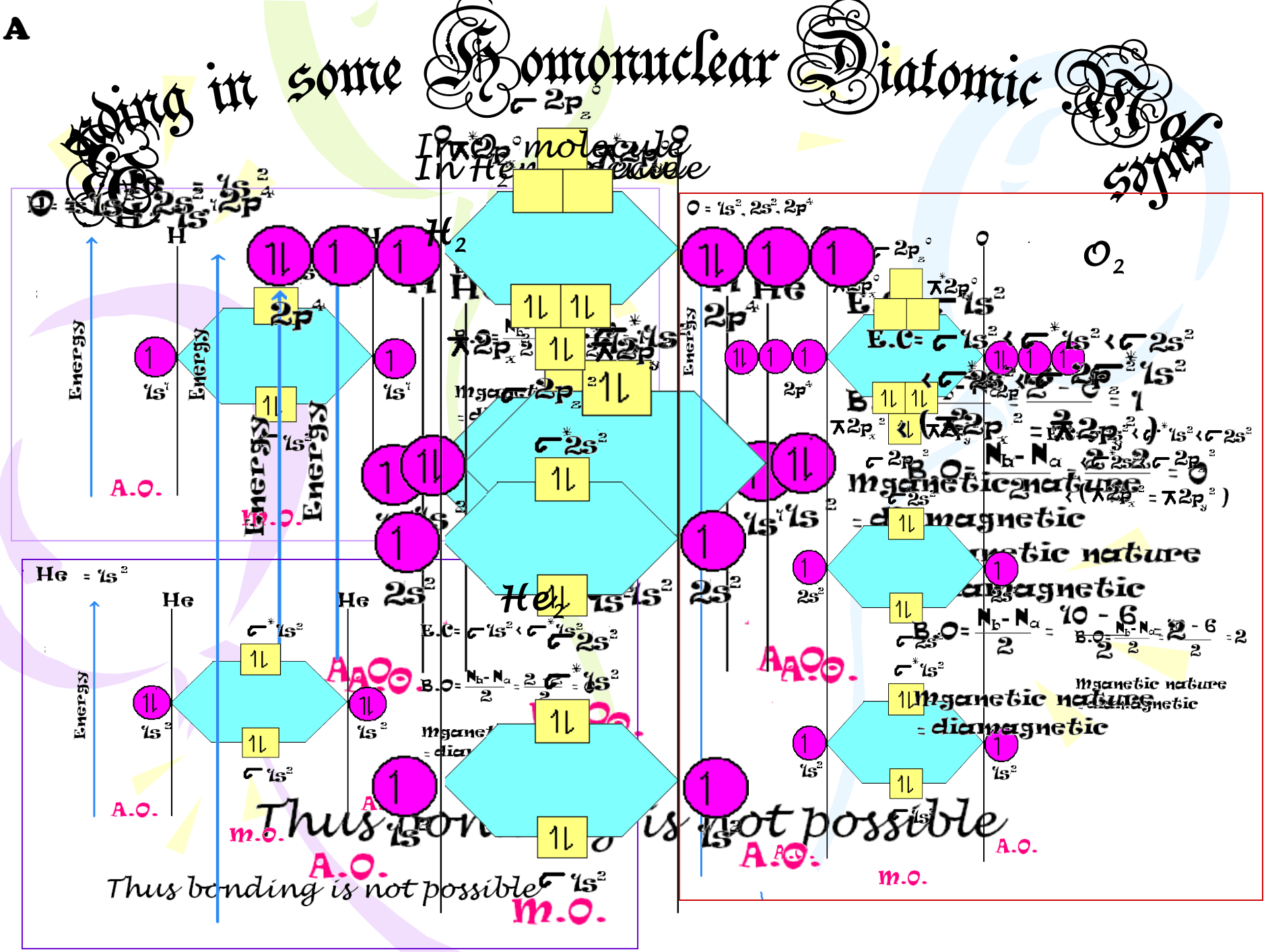
P

Molecular Orbital Theory

- The electrons in various molecules are present in molecular orbitals.
- The atomic orbitals of comparable energy and symmetry combine to form molecular orbitals.
- The molecular orbitals are polycentric.
- The no. of molecular orbitals formed is equal to the no. of atomic orbitals taking part in combination.
- The energy of the bonding molecular orbitals are less than the energy of the non bonding orbitals thus the bonding orbitals are more stable.
- The electron probability distribution around a group of nuclei in a molecule is called a molecular orbital.
- It obeys aufbau principle , Hund's rule and Puali's exclusion principle.

A

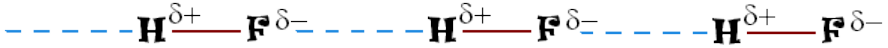
Bonding in some Homonuclear Diatomic Molecules



s

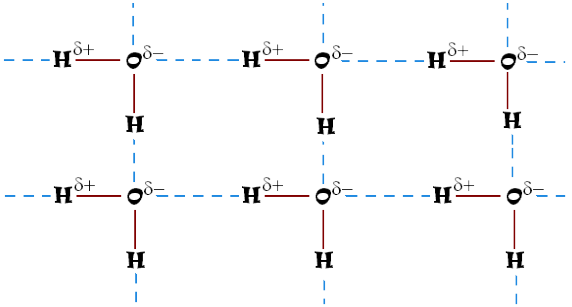
HYDROGEN BONDING

The hydrogen bond can be defined as the attractive force which binds hydrogen atom of one molecule with the electronegative atom of another molecule.



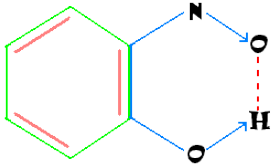
When bonded with a strong electronegative atom the hydrogen atom acquires partial positive charge as the electron gets displaced more towards the electronegative atom. This causes formation of polar molecule having electrostatic force of attraction. They can be either:-

(1)Intermolecular →



Or,

(2)Intramolecular →



The name of the slide designer is on top left corner of every slide:

A for Akarshik (rollno. 5)

S for Sayantan (rollno. 24)

P for Pratyush (rollno. 21)

Hope the project was decent……. Thanks for watching.