

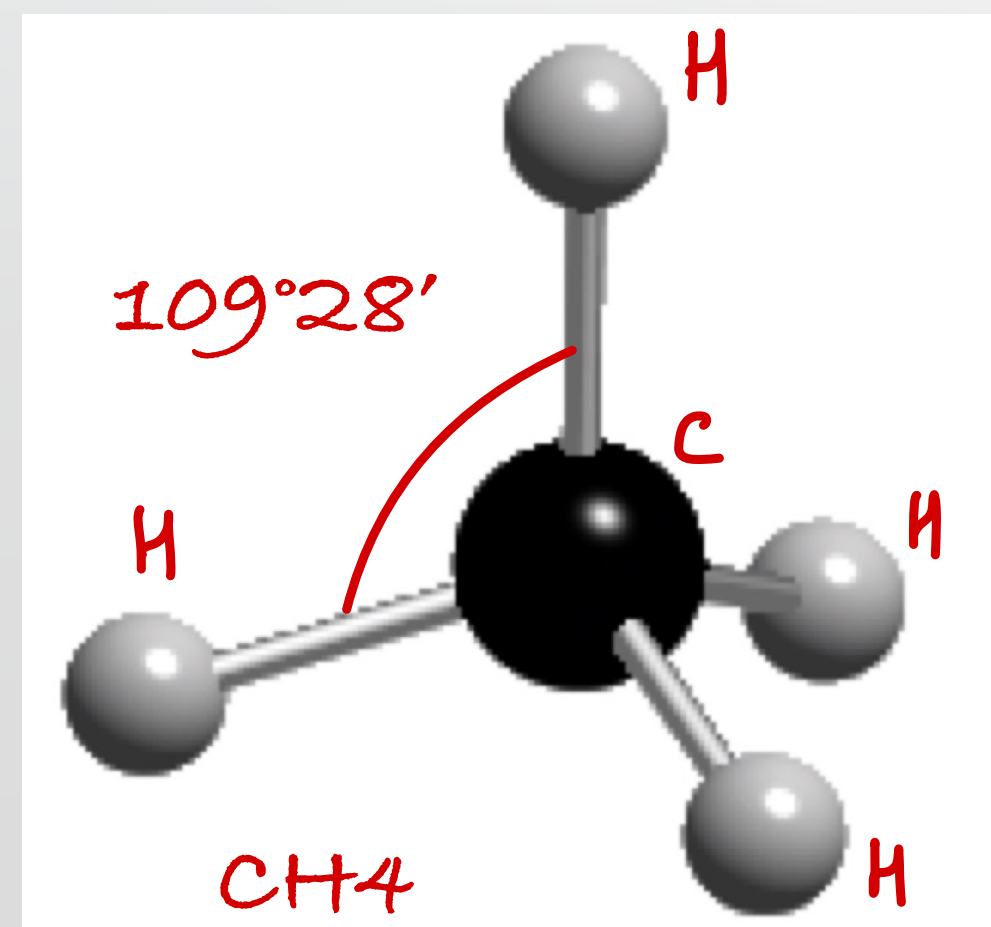
Draw backs of valence bond theory (VBT)

* valence bond theory fails to explain the structure and bonding of molecules which are poly atomic .(molecule having more than two atom.)

Let us consider the CH_4 molecule.

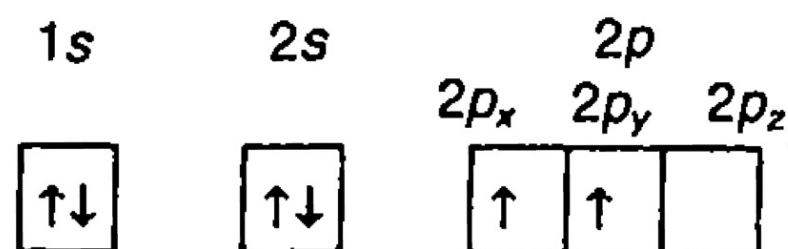
For the CH_4 molecule following observations are made.

1. All four 'C-H' bonds are identical
2. All bond are of equal strength .
3. All bond angle 'H-C-H' are equal and equal to $109^\circ 28'$

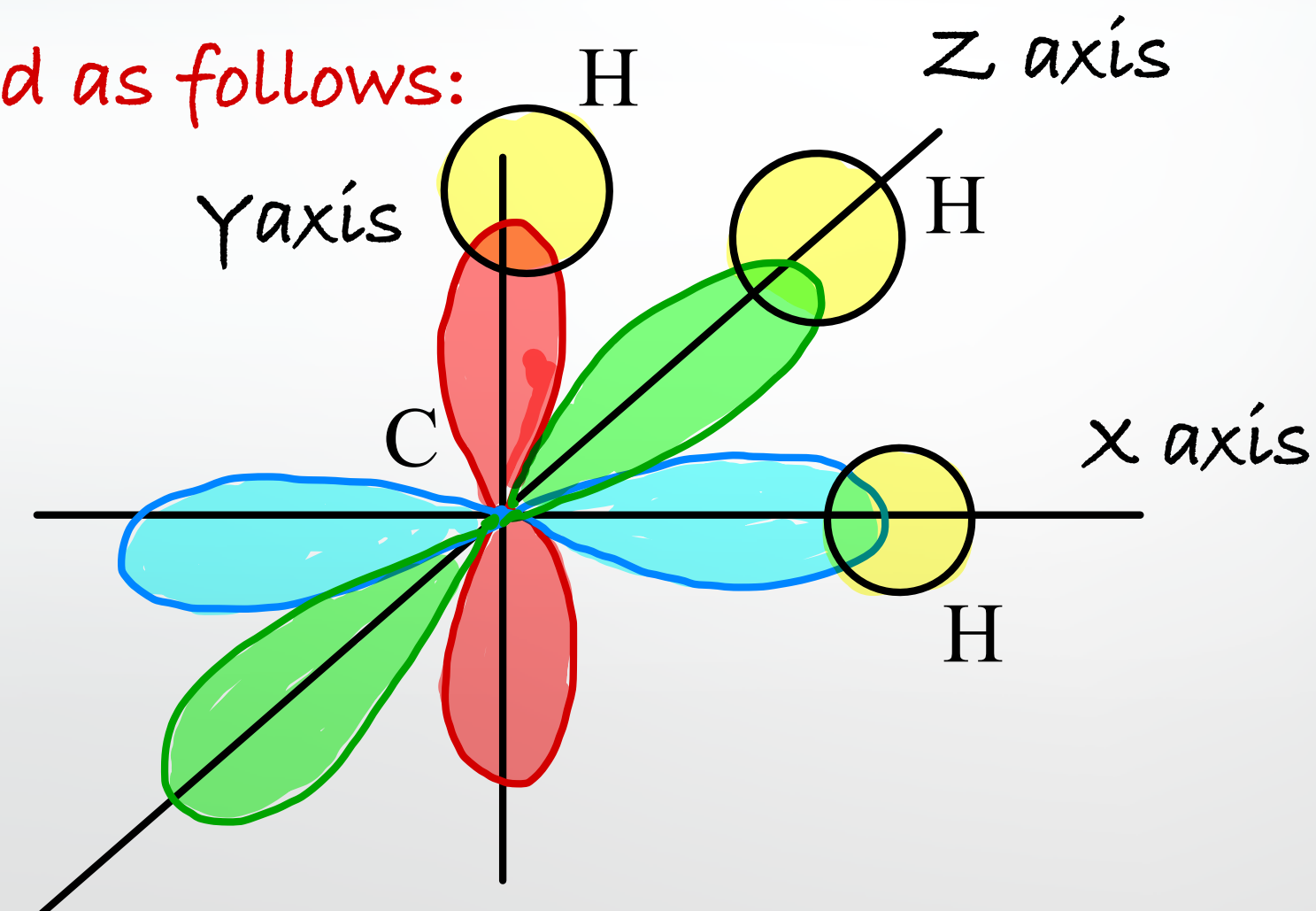
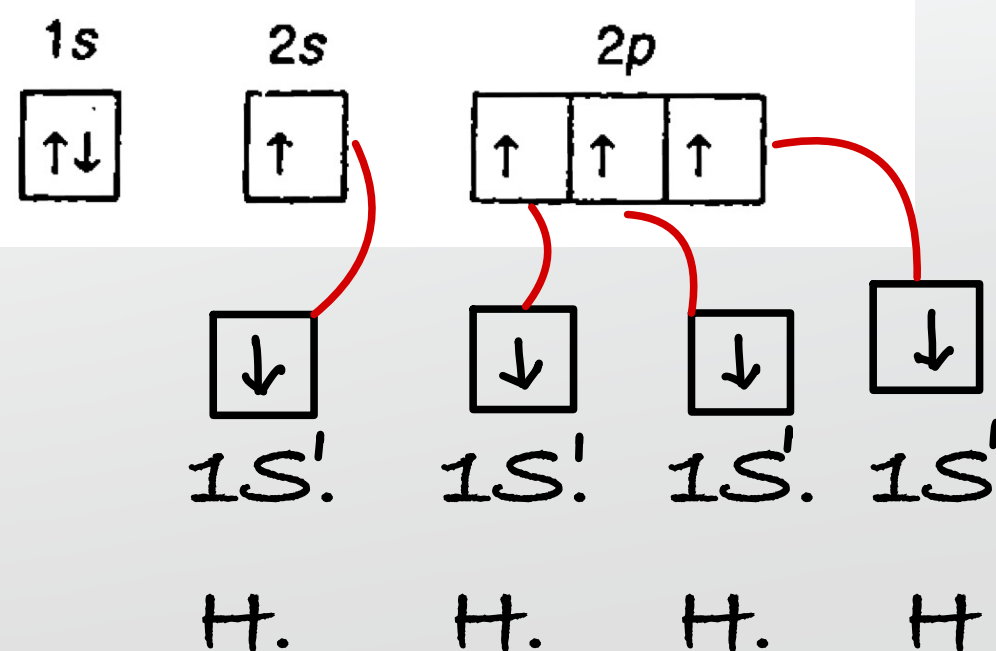


According to VBT the CH_4 molecule can be explained as follows:

Electronic structure of carbon atom – ground state



Carbon atom – excited state



If purely atomic orbitals were involved in bonding, then in the formation of methane molecule the three C–H bonds will be formed by the p – s overlap and the fourth C–H bond will be formed by the s – s overlap.

1. Two types of overlap

(a) $1s-2s$ overlap

(b) $1s-2p$ overlap

Bond strength $1s-2p > 1s-2s$

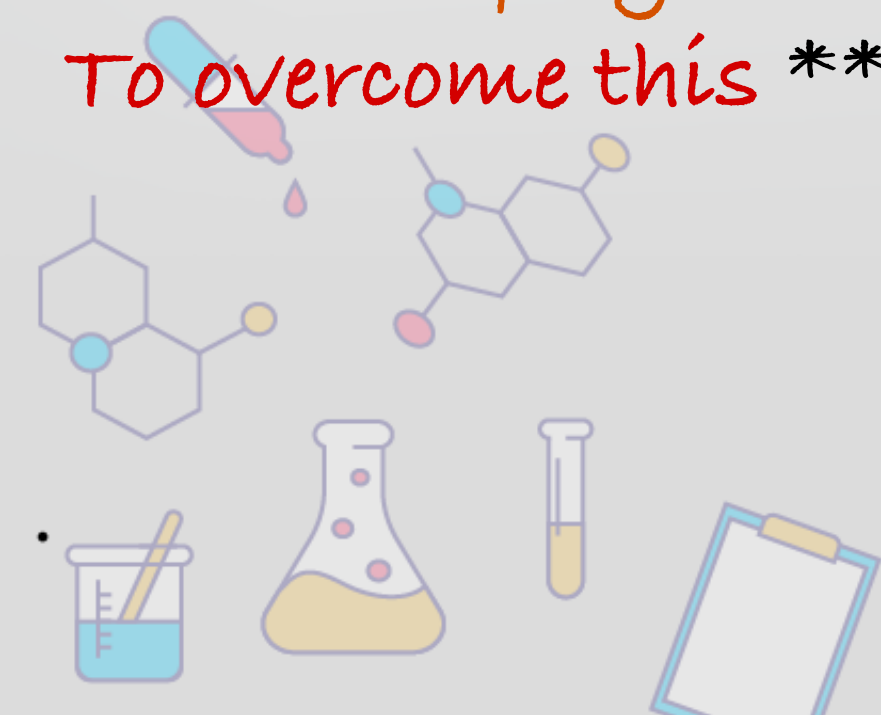
*According to VBT in CH_4 (3 ' $C-H$ ') bond should be stronger than (1 ' $C-H$ ') bond

But experimentally all ' $C-H$ ' bond are of equal strength.

*According to VBT certain bond angle in CH_4 should be 90° but in reality no bond angle in CH_4 is 90° . Instead all bond angle are $109^\circ 28'$.

*This suggest that VBT is not a good theory to predict the structure, shape of molecules which are poly atomic.

To overcome this **theory of hybridisation was introduced **



Hybridisation

Hypothetical concept

Assumption:

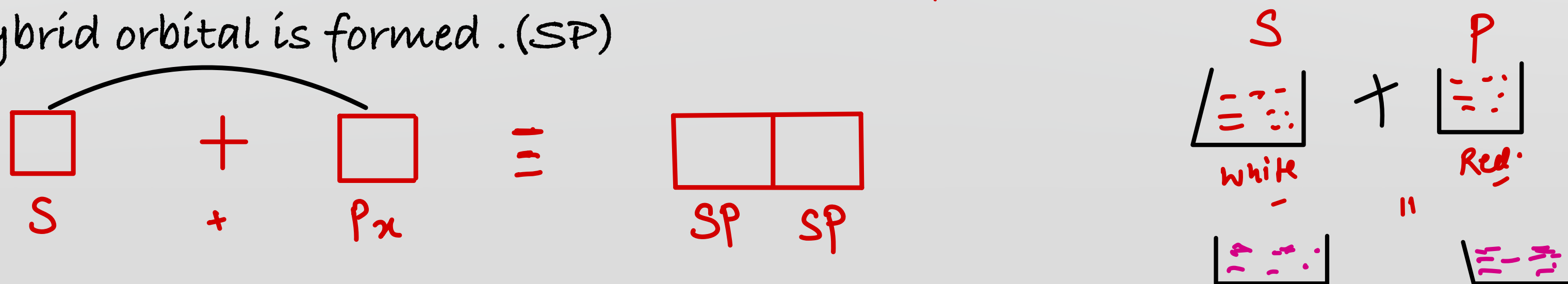
1. Atomic orbital of central atom intermix to form completely new set of hybrid orbital.
2. Mixing of atomic orbital takes place of same or nearly same energy or very less energy difference

E.g. *mixing of 2s and 2p orbital allowed*

E.g. *mixing of 2s and 3s orbital not allowed due to high energy difference.*

3. Number of hybrid orbital formed is equal to number of atomic orbital mixed.

E.g. *if intermixing of (s + p_x) i.e 2 atomic orbital takes place then 2 new hybrid orbital is formed. (sp)*

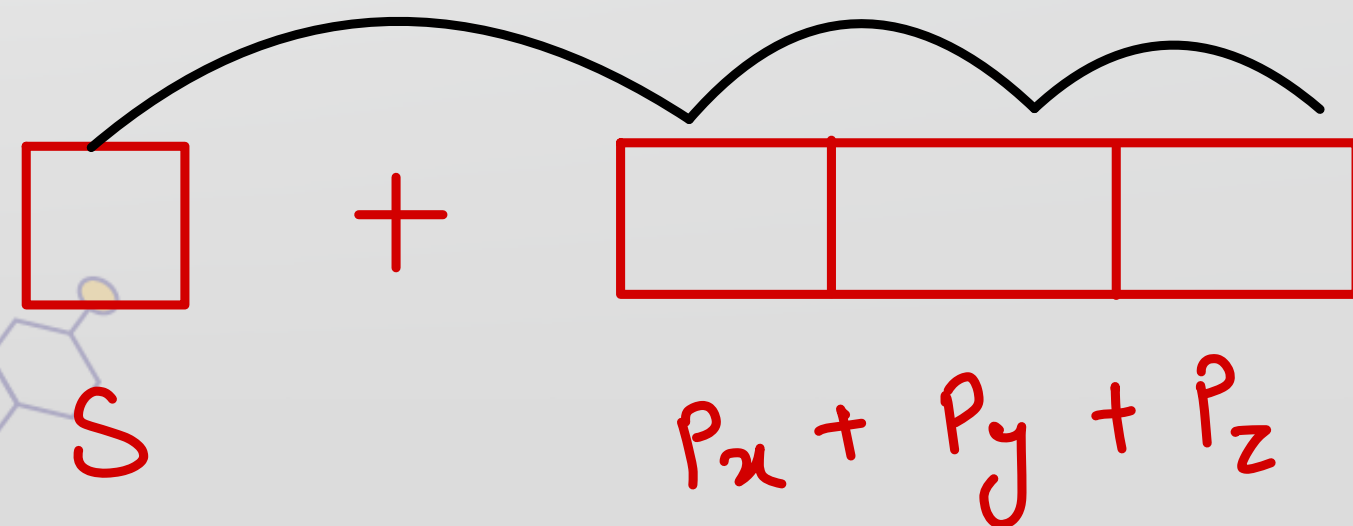
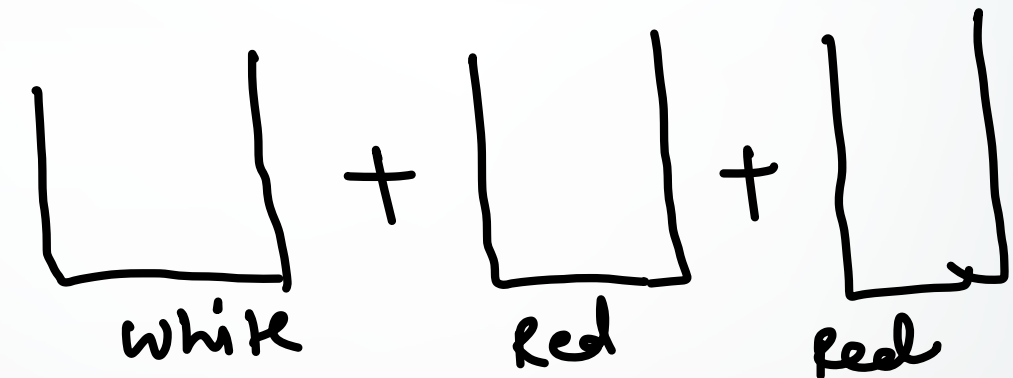
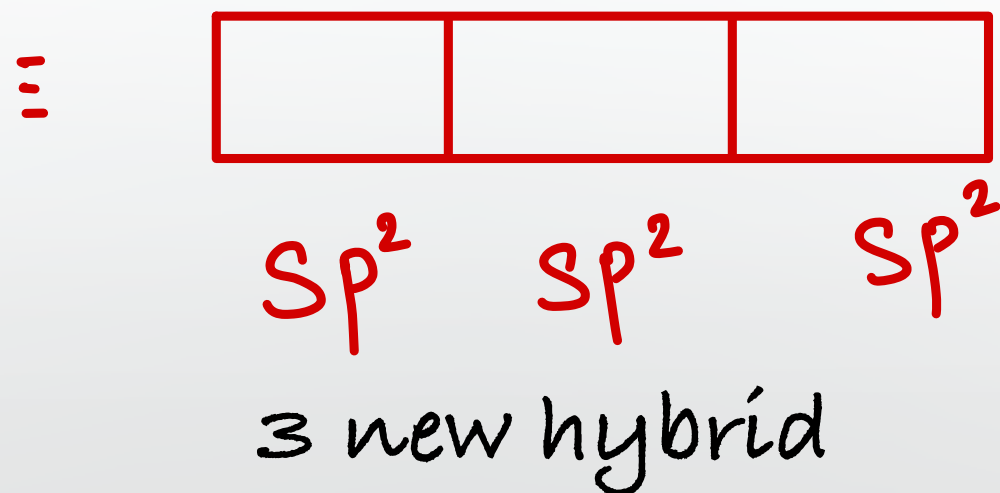
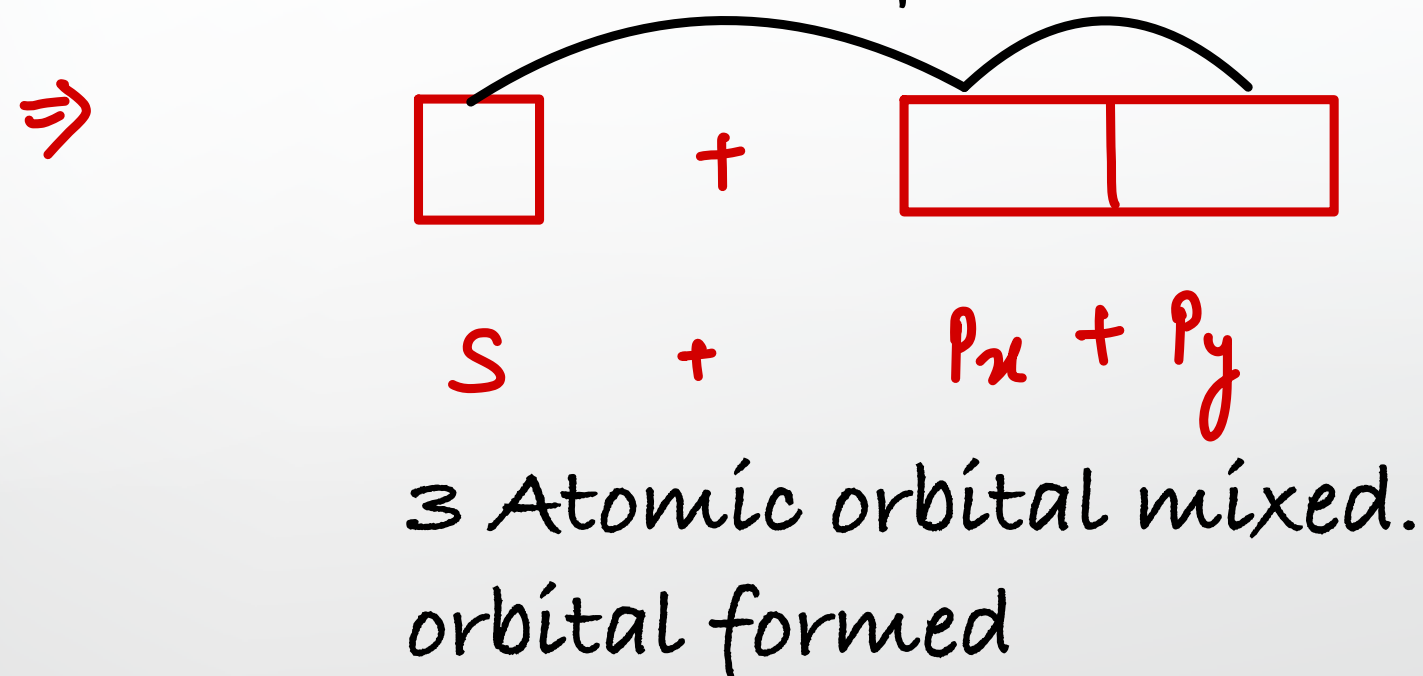


Intermixing of atomic orbital (AO)

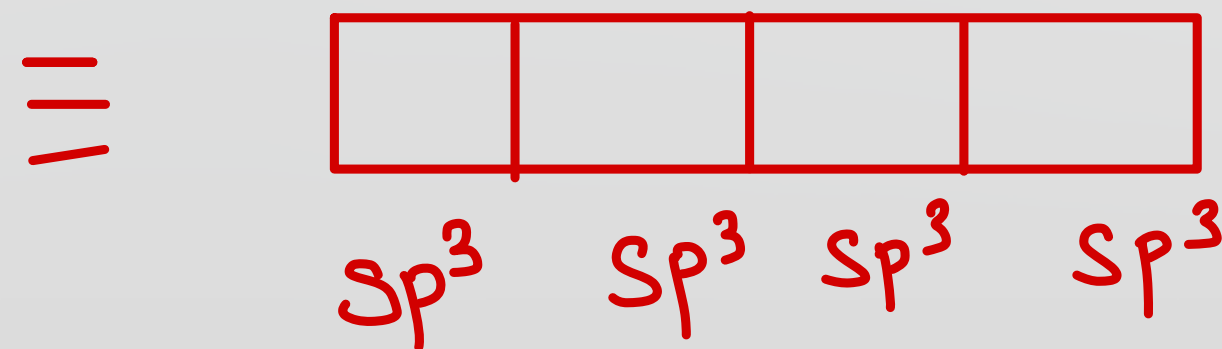
2 Hybrid orbital (H.O) formed

④ All hybrid formed is equal in size, shape and equal energy.

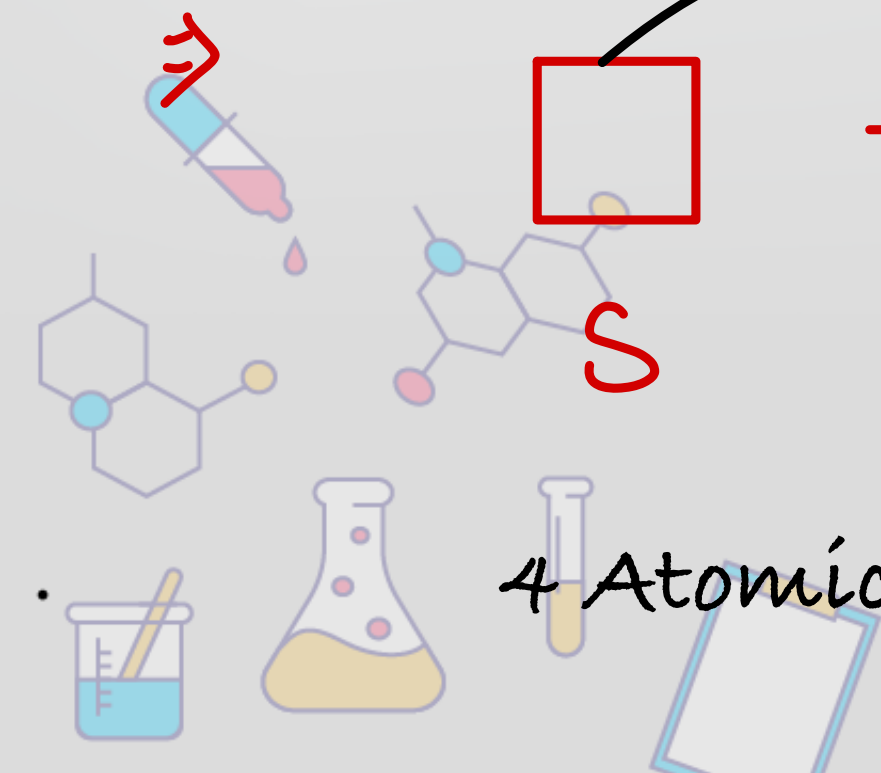
Some more example:



4 Atomic orbital mixed.



4 Hybrid orbital formed



Thus hybridization may precisely be defined as the phenomenon of mixing up (or merging) of orbitals of an atom of nearly equal energy, giving rise to entirely new orbitals equal in number to the mixing orbitals and having same energy contents and identical shapes.

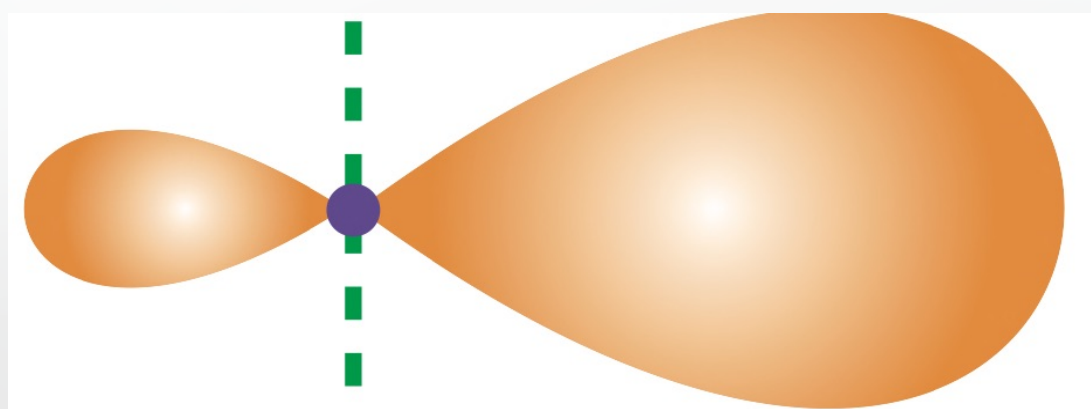
Note 1. Hybridisation occurs first then overlapping takes place

2. Hybridisation is mixing of atomic orbital and not electron hence fully filled half filled or empty orbital can participate.



Features of hybrid orbital

- * The shape of each hybrid orbital is such that one lobe is small and the other lobe is large
- * Overlapping always occur by bigger lobe as it has 98% probability of having electron



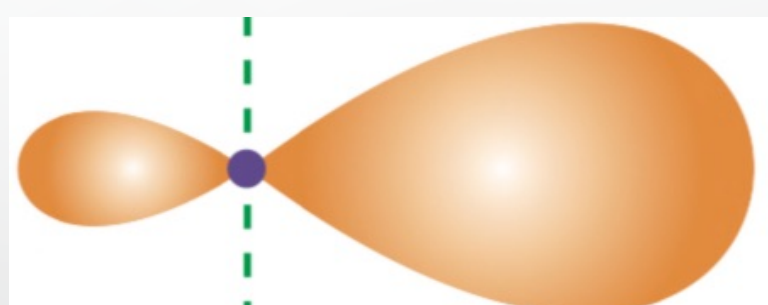
Smaller lobe. Larger lobe

Hybrid orbital

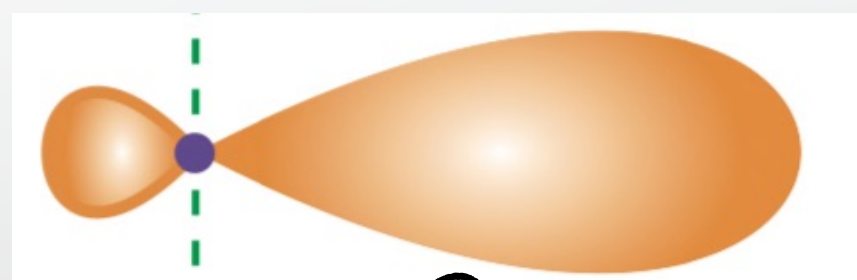


* Hybrid orbitals have same shape but different size. Size of hybrid orbital depends upon % s character.

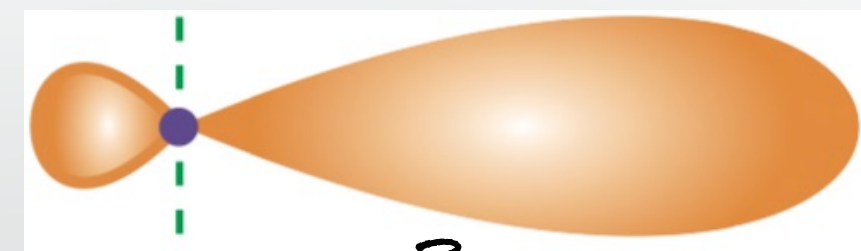
* As the % s character increases in a hybrid orbital, the hybrid orbital becomes bulkier and shorter. On the other hand as the % p or % d character increases, the orbital becomes longer and thinner.



sp



sp^2



sp^3

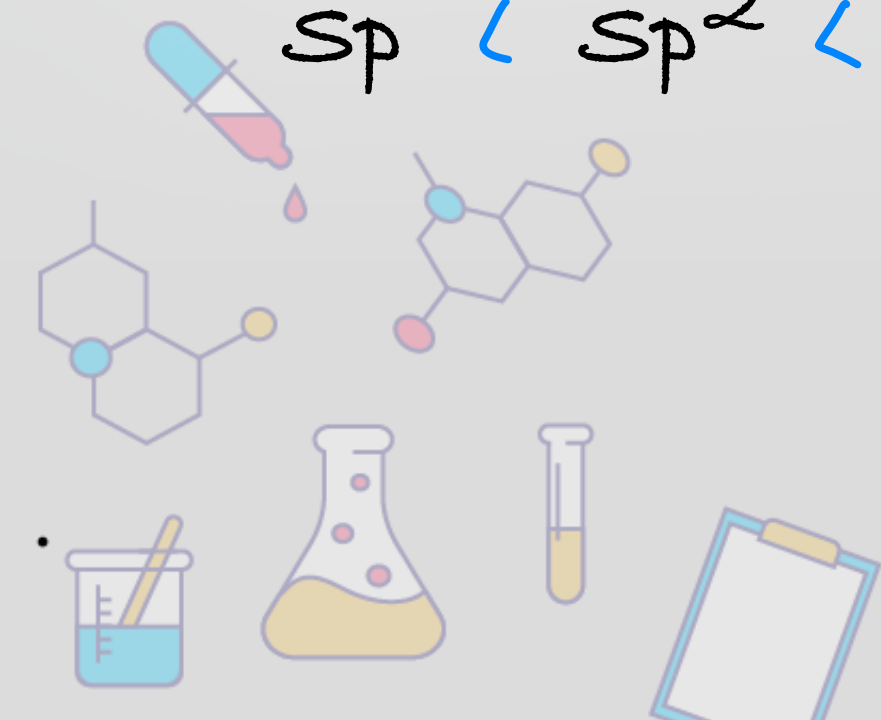
Order of size and energy

$sp < sp^2 < sp^3$

sp % s character = 50%
% p character = 50%

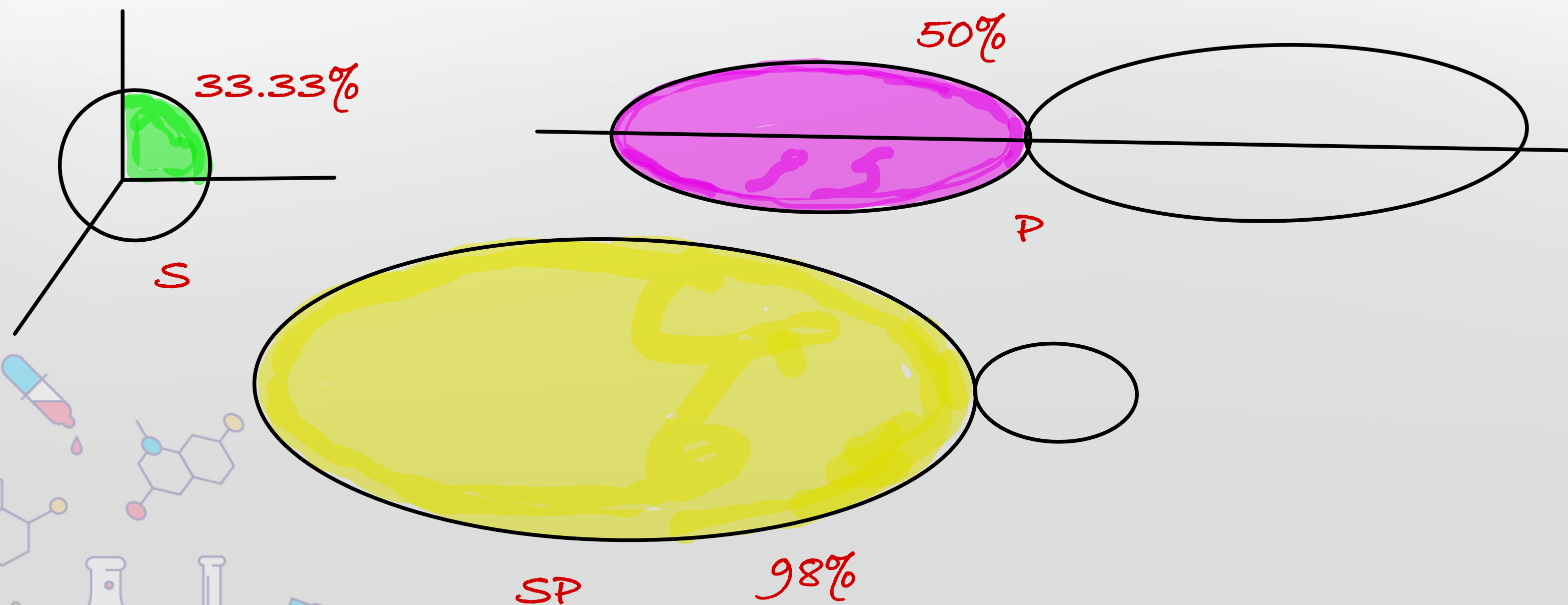
sp^2 % s character = 33.33%
% p character = 66.67%

sp^3 % s character = 25%
% p character = 75%

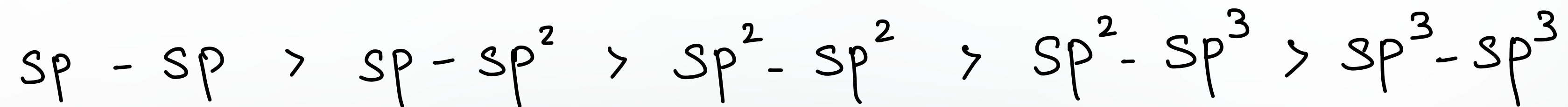


*All hybrid orbital has directional property and more directional property than atomic orbital.

*Hybrid orbital has more directional property because it has 98% of finding electron
 $S-S. < S-P. < P-P. < S-SP.$ more directional nature more strength

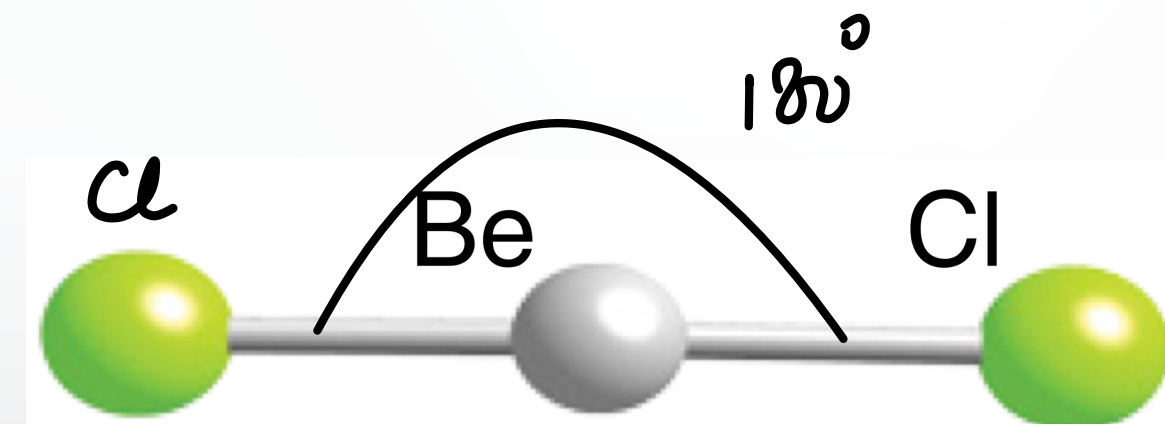
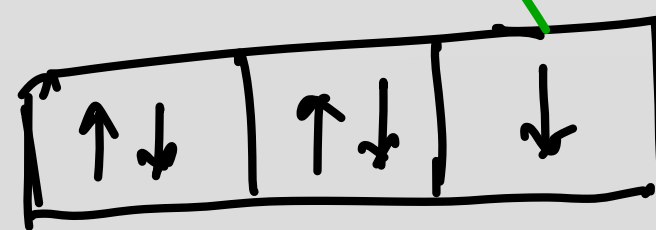
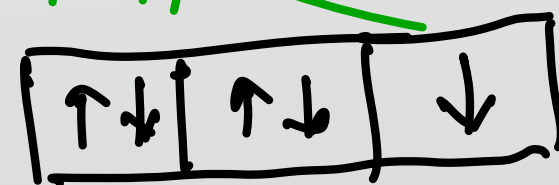
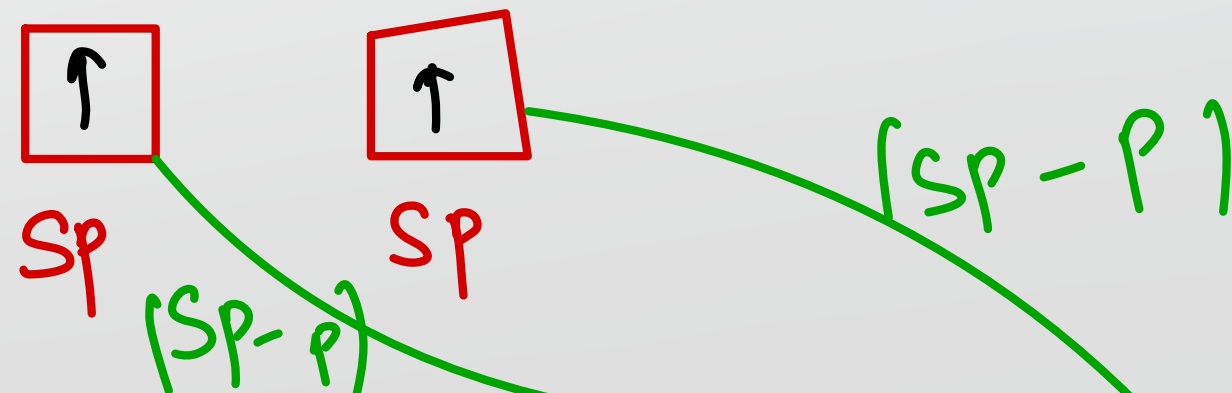
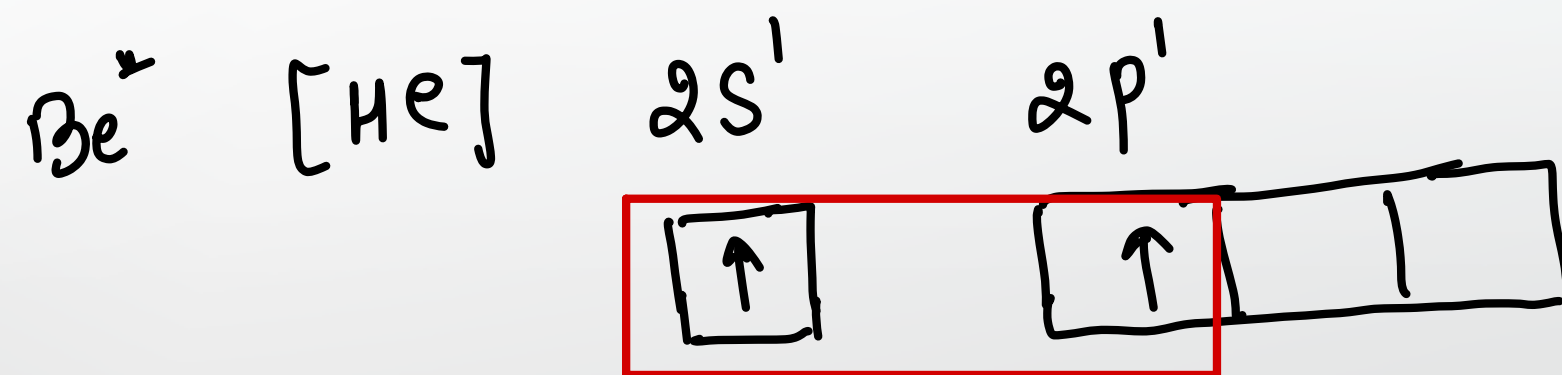


Bond strength of hybrid orbital directional proportional to %s character



(Q) Applying concept of hybridisation in BeCl_2 (g) molecule

Be [He] $2s^2$



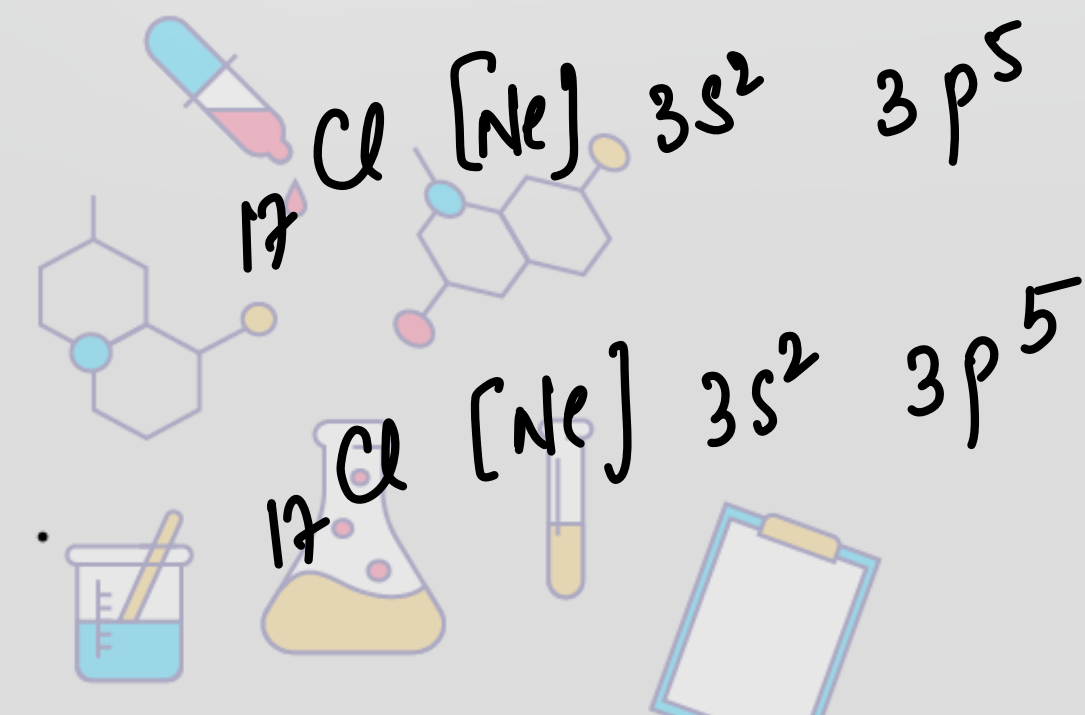
Geometry/Shape: linear

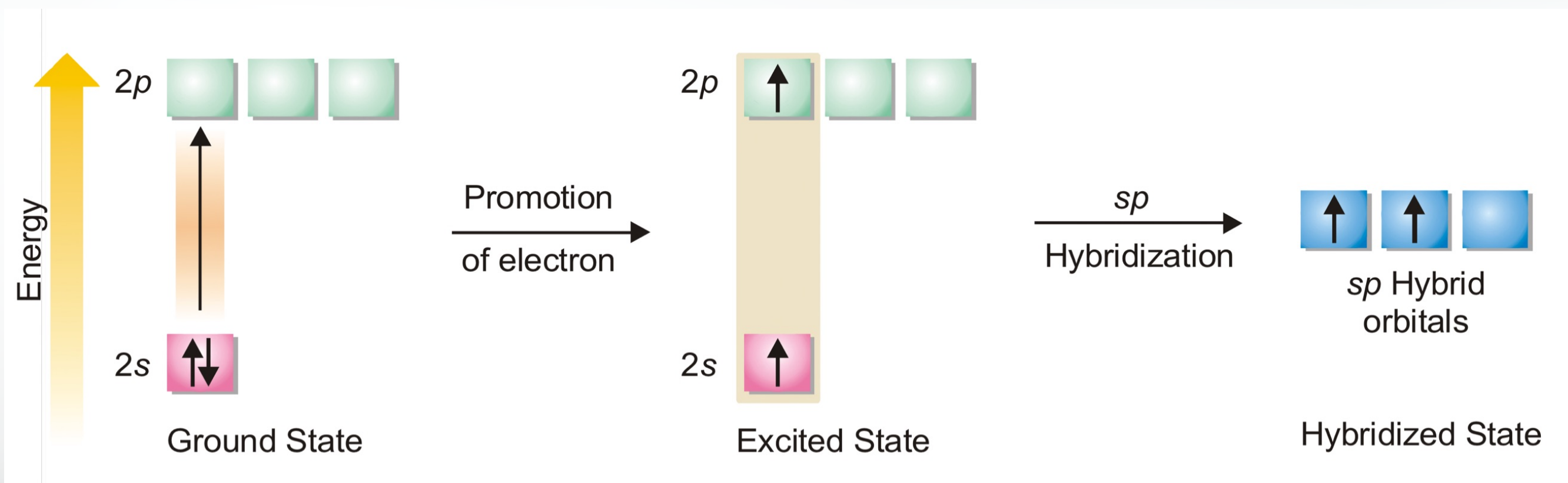
Number of atom in one plane = 3

Bond Angle (B.A) = 180°

Planar molecule

Hybridization (C.A) = sp



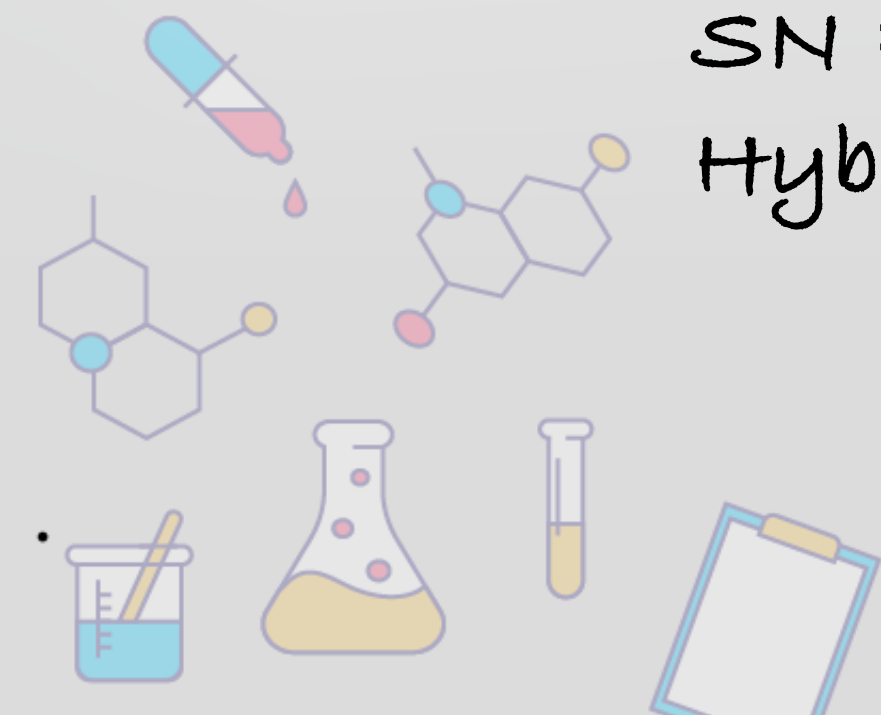


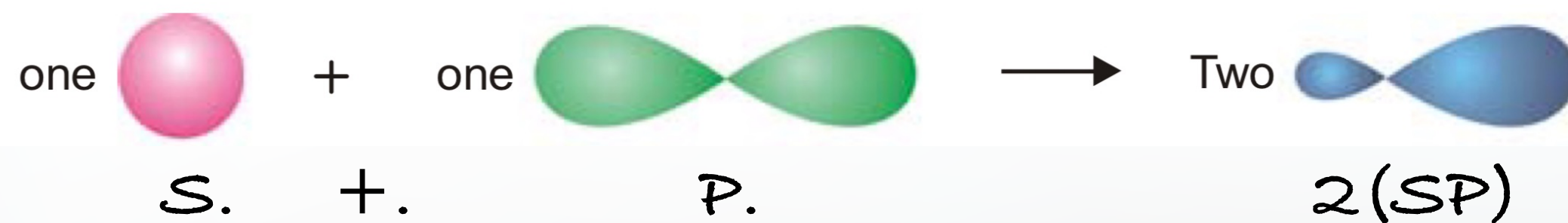
Total hybrid orbital (T.H.O) / steric No. (S.N) = number of sigma bond + lone pair on C.A

Example 1 : BeCl2

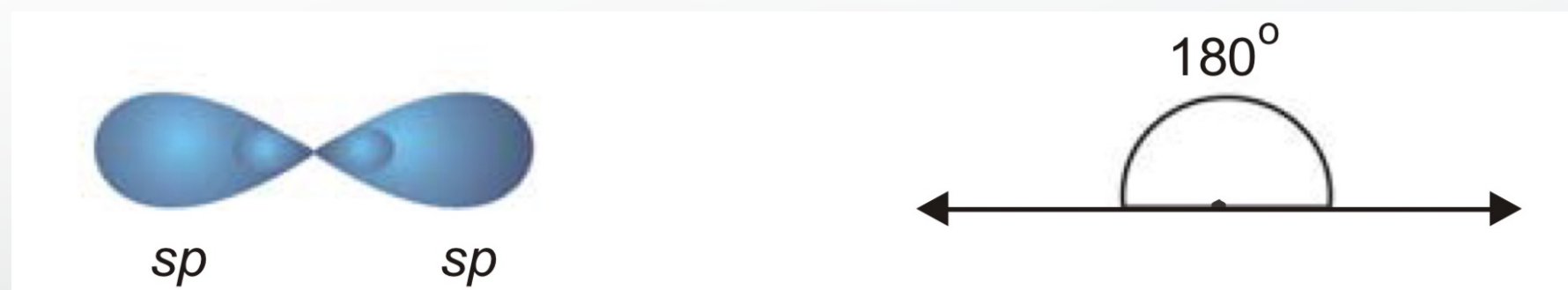
$$SN = 2 + 0 = 2$$

Hyb : sp

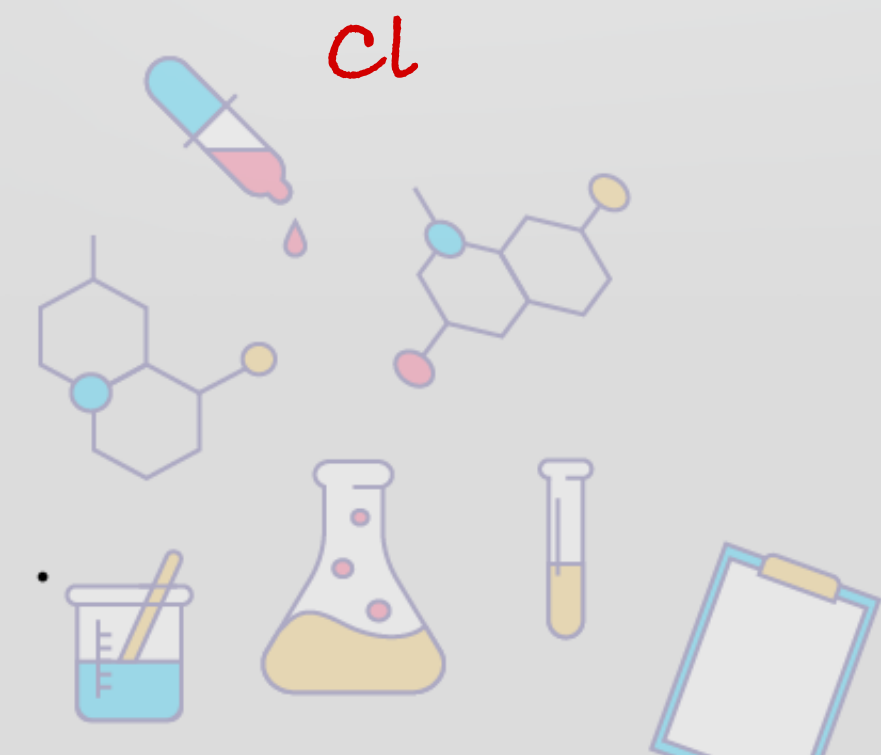
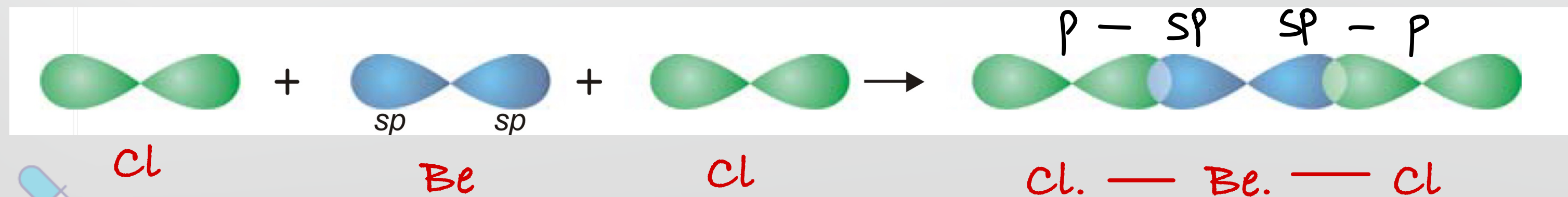




Intermixing of A.O to form H.O



Arrangement of H.O to minimise electronic repulsion



(Q) Apply concept of hybridisation in BF_3 (g) molecule

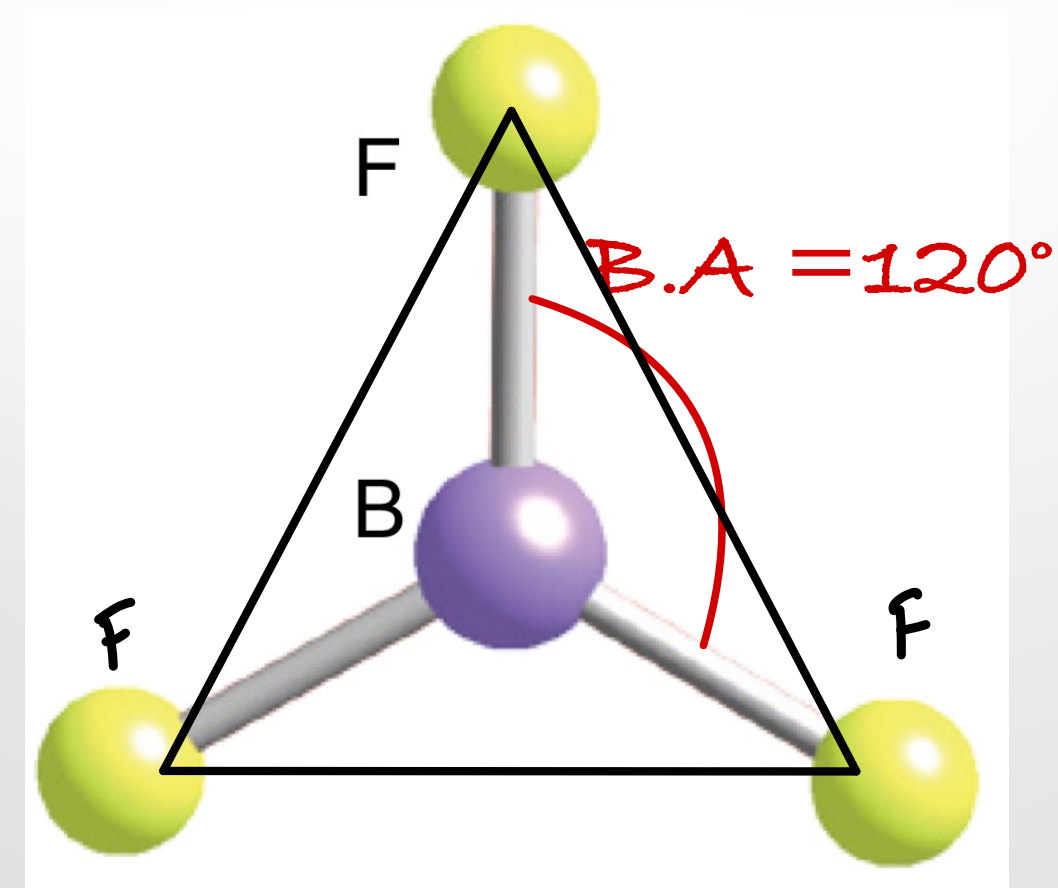
Short trick:

$$\text{THO / SN} = \sigma \text{ bond} + \text{LP}$$

$$= 3 + 0$$

$$= 3$$

Hyb: sp^2

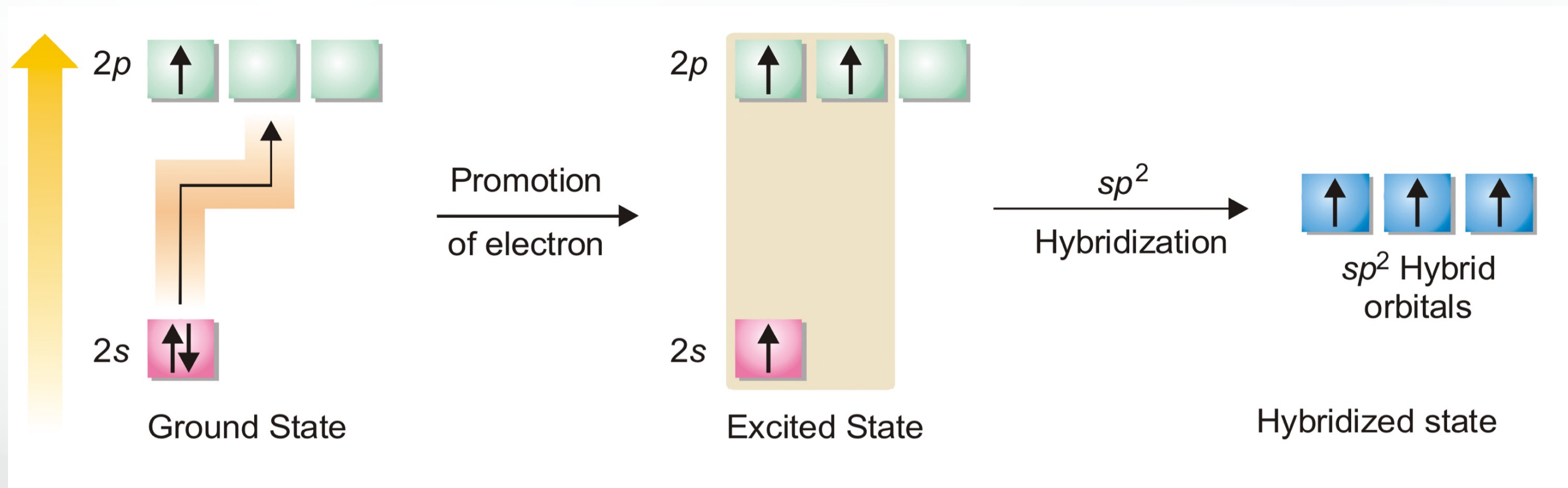


Shape: Trigonal planar

Max. Number of atom in one plane = 4

Planar molecule



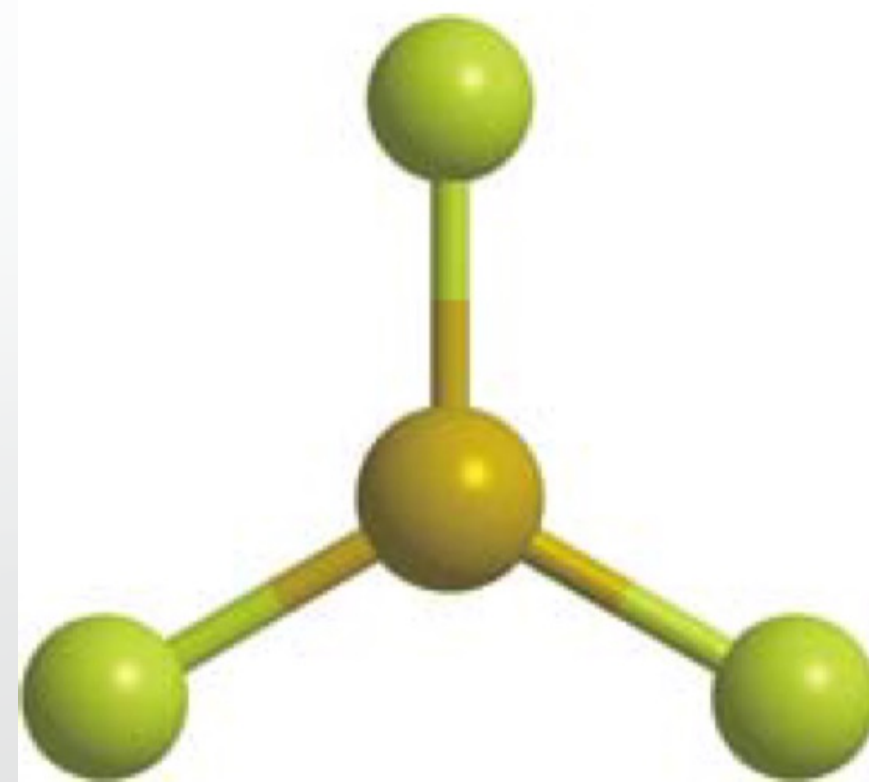
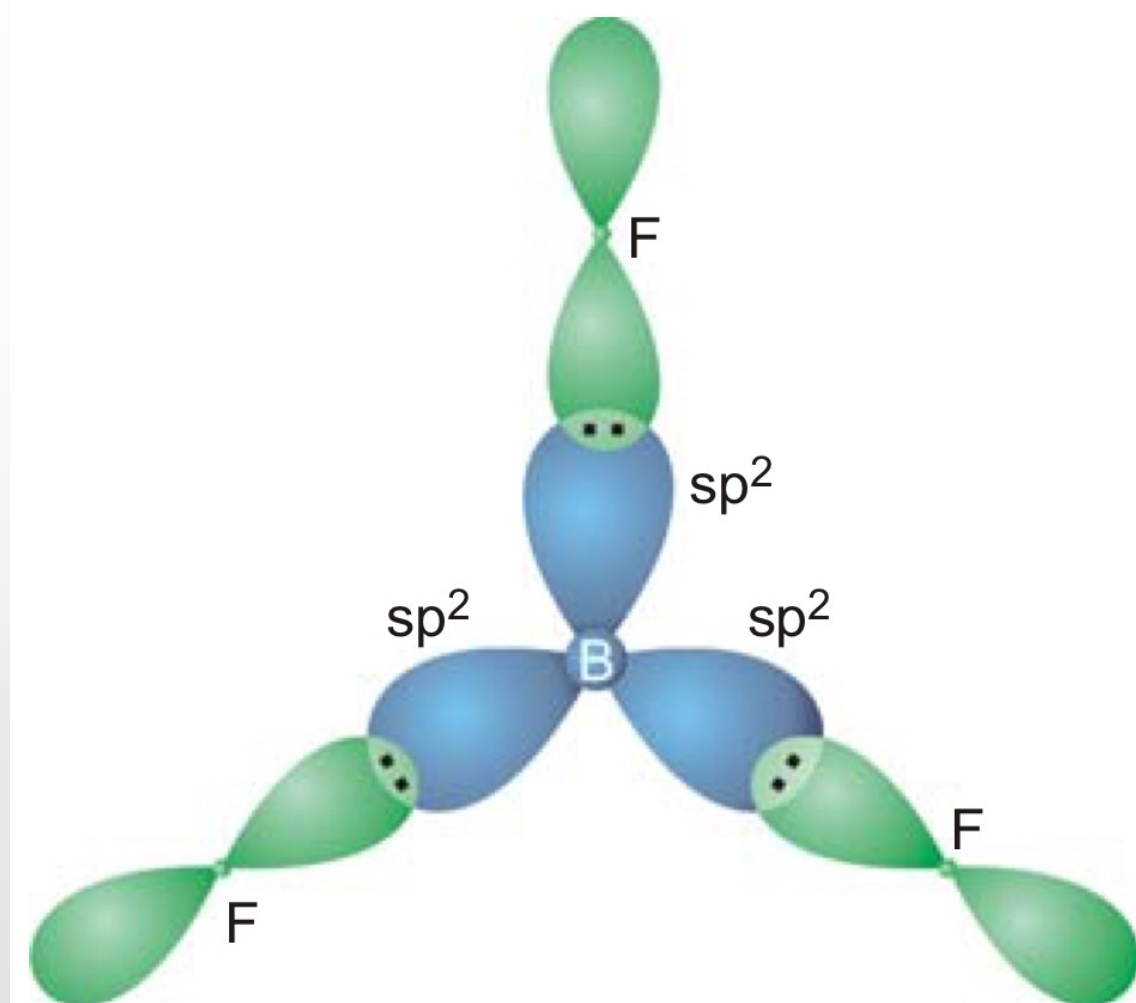


Example 2 : BF_3

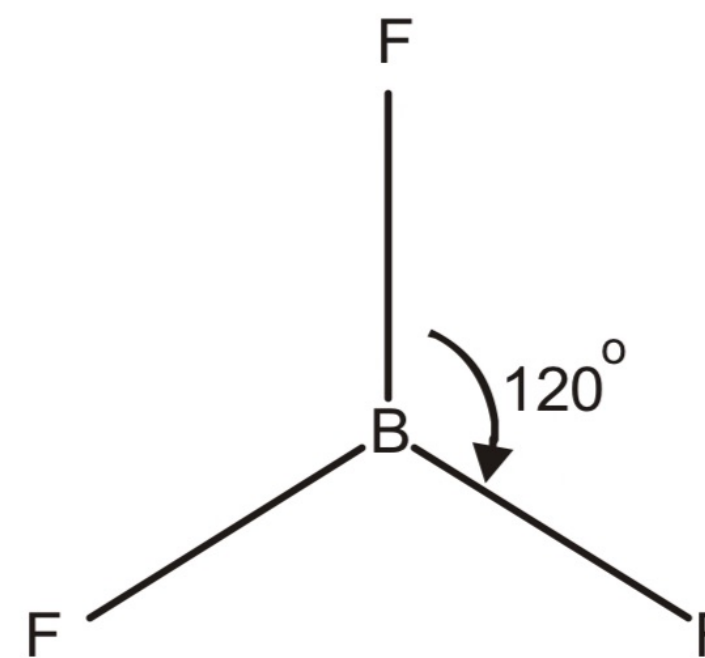
$$\text{SN} = 3 + 0 = 2$$

Hyb : sp^2

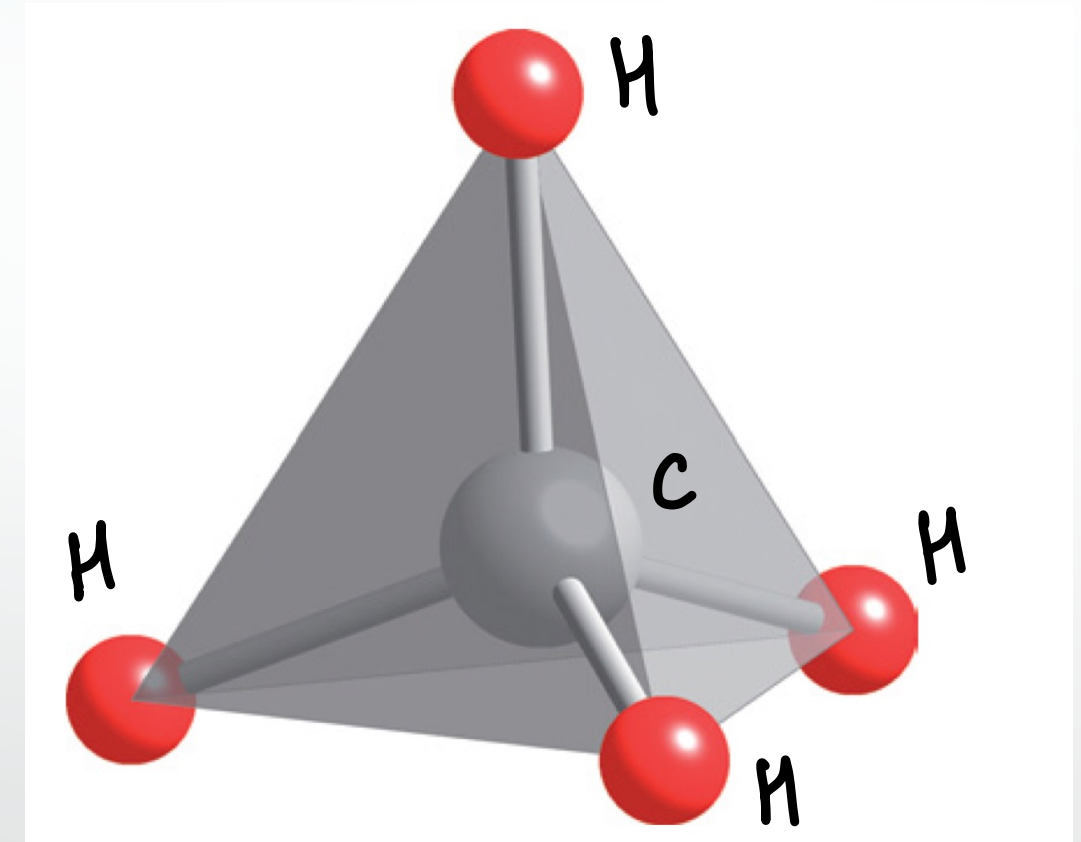




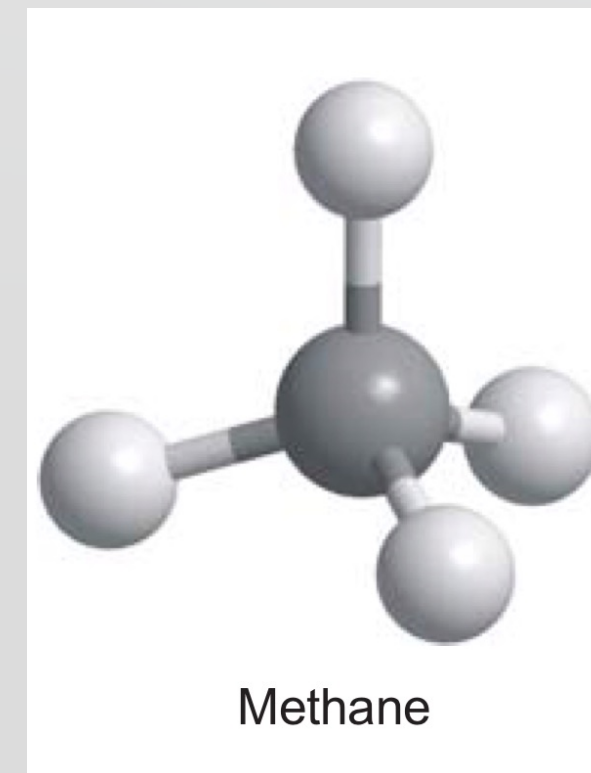
Boron trifluoride



(Q) Apply concept of Hybridisation in CH_4 molecule.



Shape : Tetrahedral



Methane

Non planar

