Factors affecting bond angle

(a) State of Hybridisation
(b) Presence of lone pair
(c) Electronegativity of central atom
(d) Electronegativity of surrounding atom
(e) Size of surrounding atom
(f) Lone pairs may sometimes be transferred from a filled shell of one atom to an unfilled shell of another bonded atom, causing less repulsion.
(g) Multiple bond orbital repel other orbitals more strongly than single bond orbitals.

Chemical Bonding

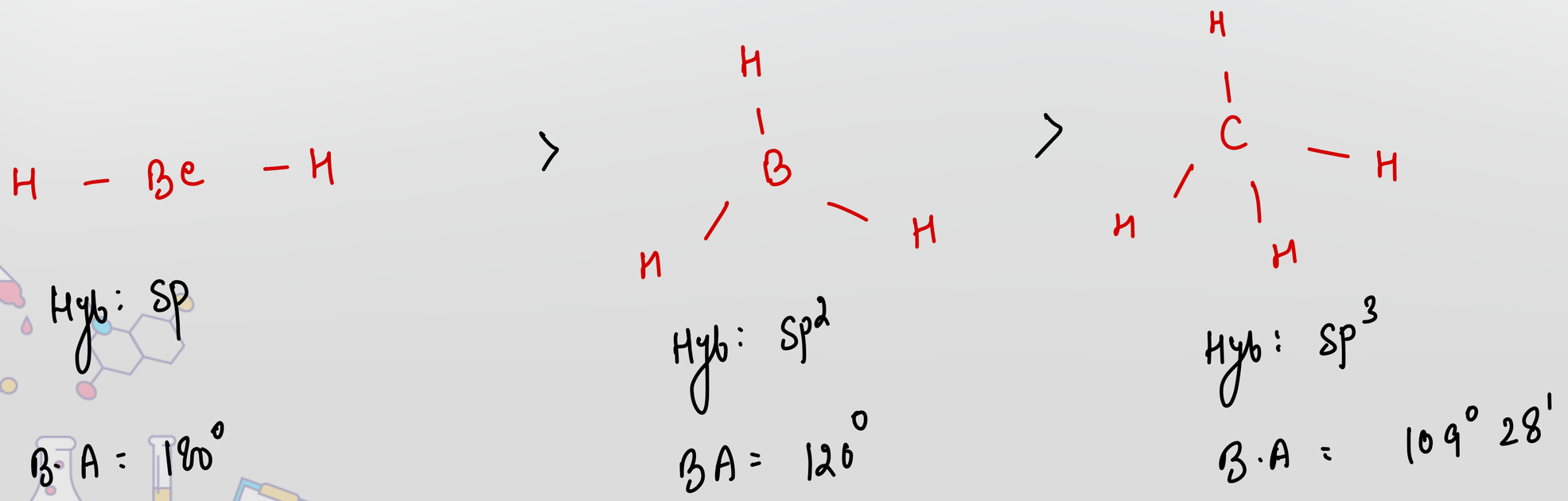
Steps to compare bond angle

Check the hybridisation of C.A

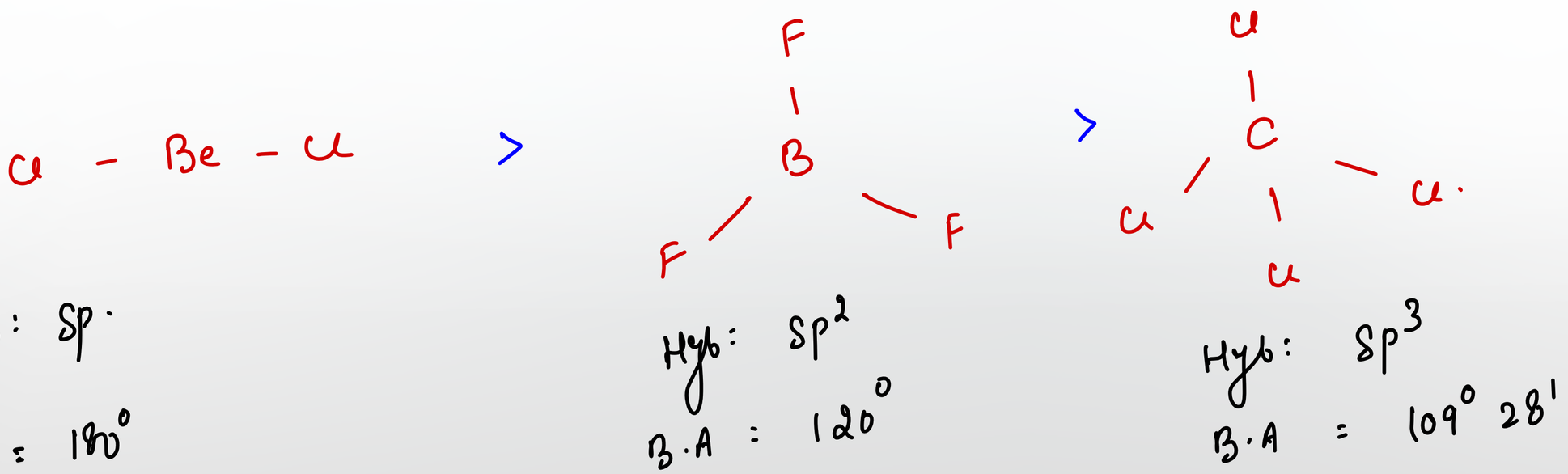
STEP1

Hybridisation state of central atom: Compounds having different hybridisation have diferent bond angle.

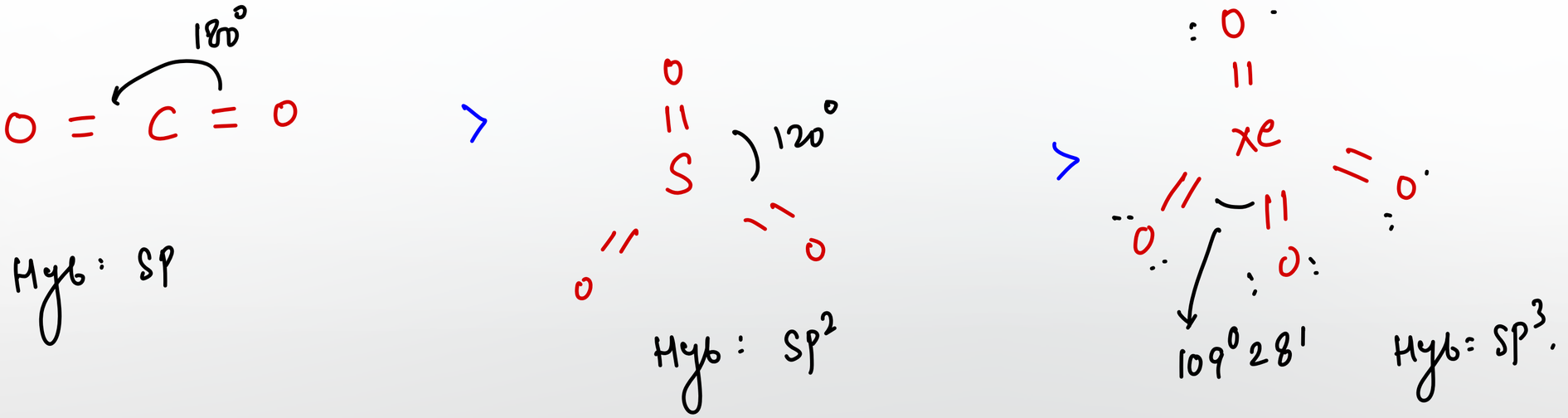
Ex.	BeH_2	BH_3	CH_4
Hybridisation	sp	sp^2	sp^3
Bond angle	180°	120°	109°28'



(Q) compare bond angle of the given molecule (a) BeCl2 (b) BF3. (C) CCl4



(Q) compare bond angle between (a) CO2 (b) SO3. (C). XeO4

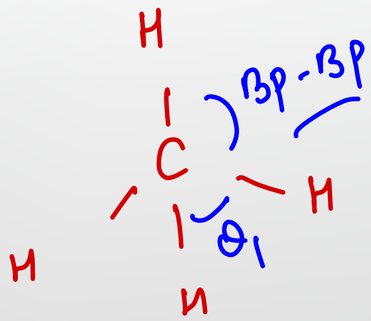


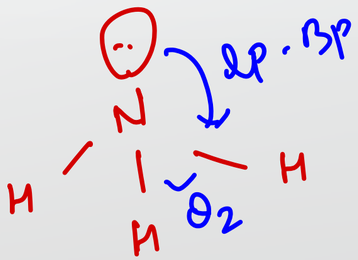
** what if the hybridisation is same for all the molecule ?

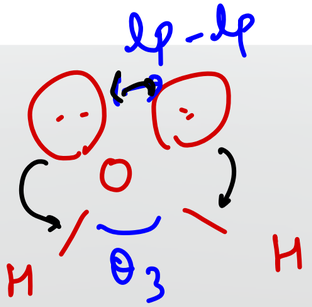
STEP 2

Lone pair of electron: If compounds have same hybridisation states then bond angle depends on lone pair of electron.

Ex.	CH_4	NH_3	H_2O
Hybridisation	sp^3	sp^3	sp^3
Lone pair e^-	zero	one	two
Bond angle	109°28'	107°	105°







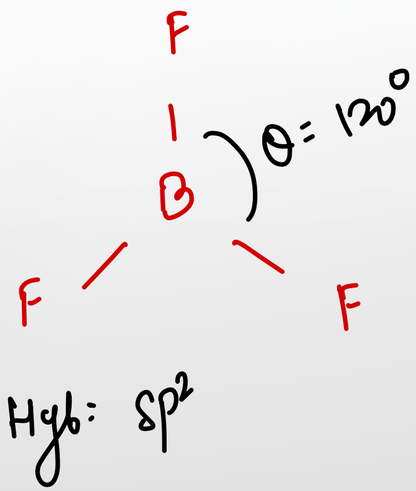
$$\theta_1 > \theta_2 > \theta_3$$

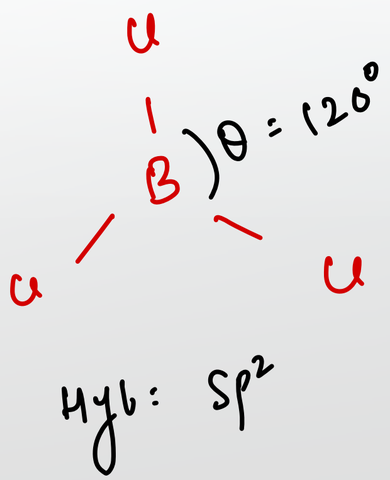
The different in bond angle is explained on the basis of following repulaion sequence
The repulsion between

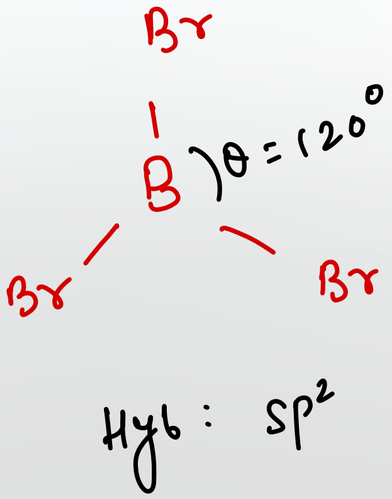
lone pair-lone pair > lone pair - bonded pair > bonded pair - bonded pair

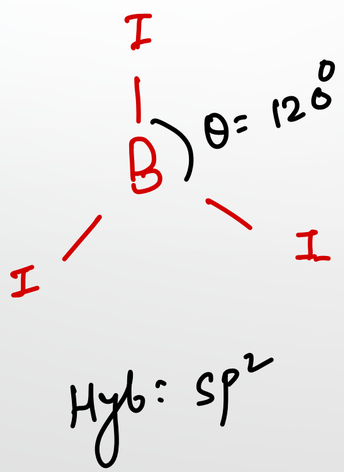
(Q) How to compare bond angle if hybridisation is same and there is no lone pair on central atom.?

Compare bond angle in BF_3 , BCl_3 , BBr_3 , BI_3









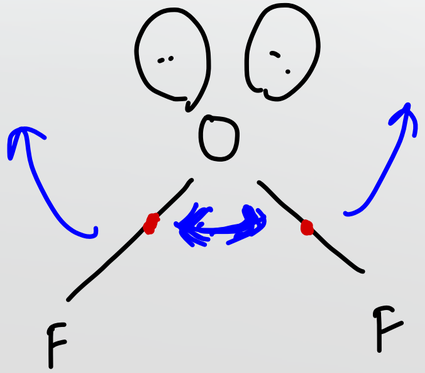
(Q) How to compare bond angle when hybridisation is same and number of lone pair on central atom is also same?

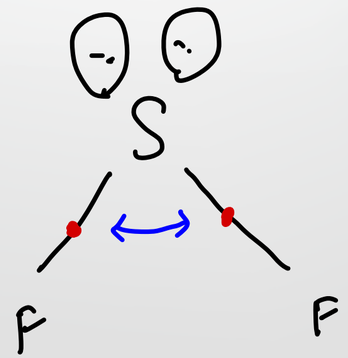
Step 3:

Electronegativity: When compounds having same hybridisation state of central atom and same number of lone pair of electrons, then bond angle depends on electronegativity.

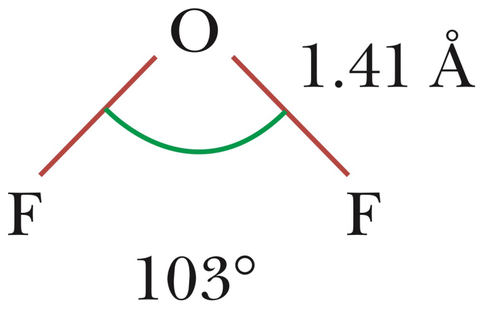
Bond angle $\propto$ electronegativity of central atom

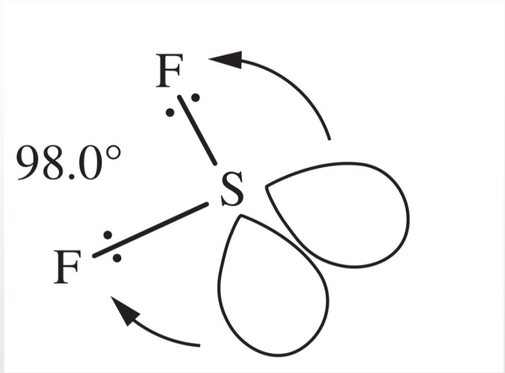
Compare bond angle in (a) OF_2 and (b) SF_2



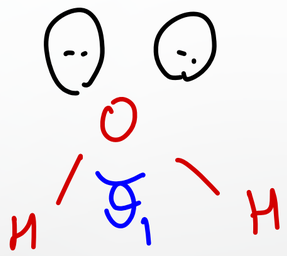


* Hyb: sp^3 Hyb: sp^3
* no of lone pair = 2 (same)

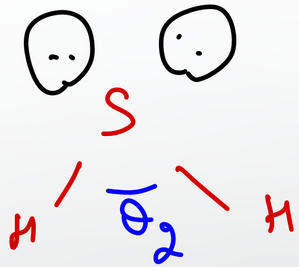

O
1.41 Å
F
F
103°


F
98.0°
S
F

(Q) Compare bond angle in (a) H2O and H2S
(b) NH3 and PH3



Hyb: sp^3



Hyb: X

$\theta_1 > \theta_2$

Hyb: sp^3

$\theta_1 > \theta_2$

Drago's rule

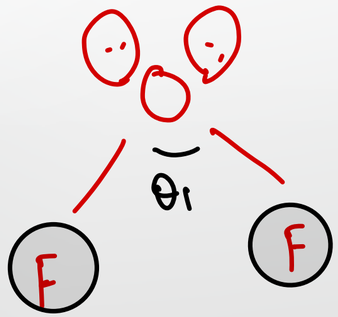
(Q) How to compare bond angle if hybridisation is same ,number of lone pair is same and Central atom is also same

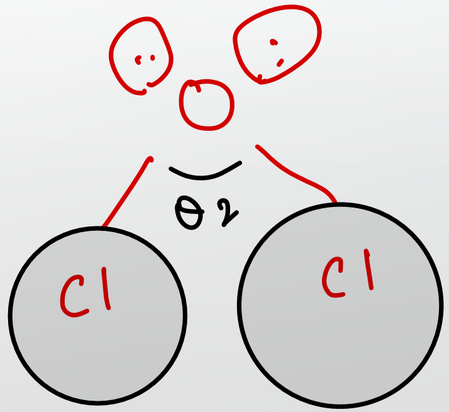
Step 4

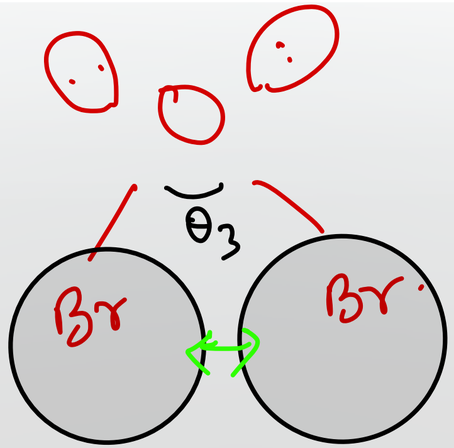
Size of terminal atoms: When size of terminal atoms increases, bond angle increases.

Ex. $OF_2 < Cl_2O < Br_2O$

$PF_3 < PCl_3 < PBr_3$







$\theta_3 > \theta_2 > \theta_1$

Steric repulsion

Hyb: sp^3

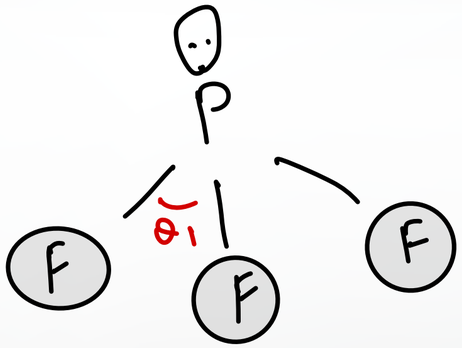
Hyb: sp^3

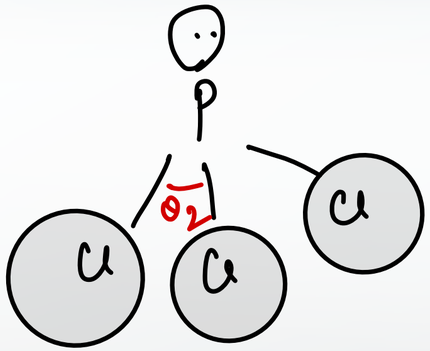
Hyb: sp^3

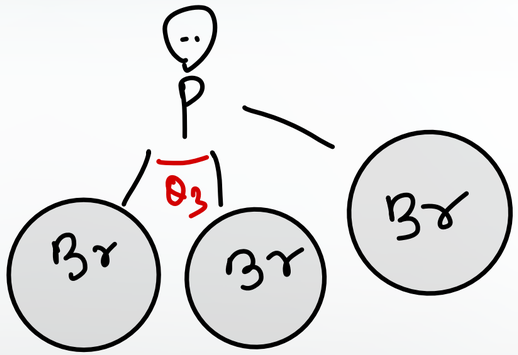
no of lone pair : 2 in all cases

⇒ CA :- Same.

Chemical Bonding



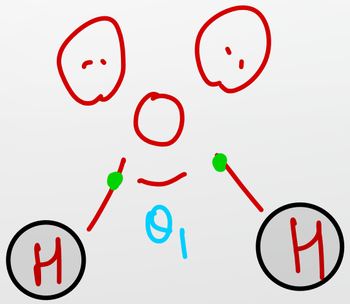


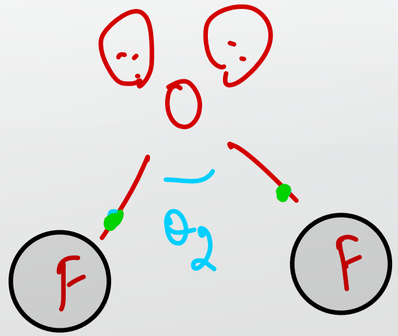


$$\theta_3 > \theta_2 > \theta_1$$

** Special case bond angle.

(Q) compare bond angle in H2O and OF2





Hyb: sp^3

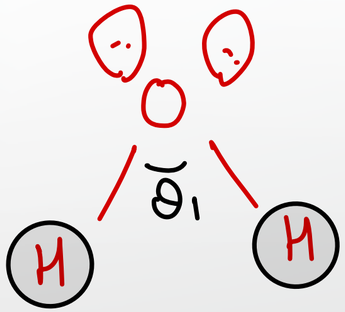
no of lp: Same

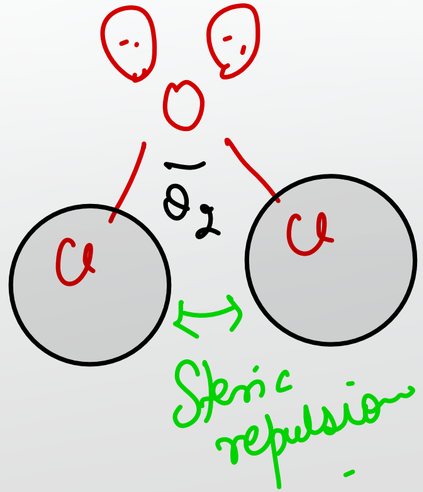
CA: Same

SA: Size Small

$\theta_1 > \theta_2$

(Q) compare bond angle in H2O and OCl2





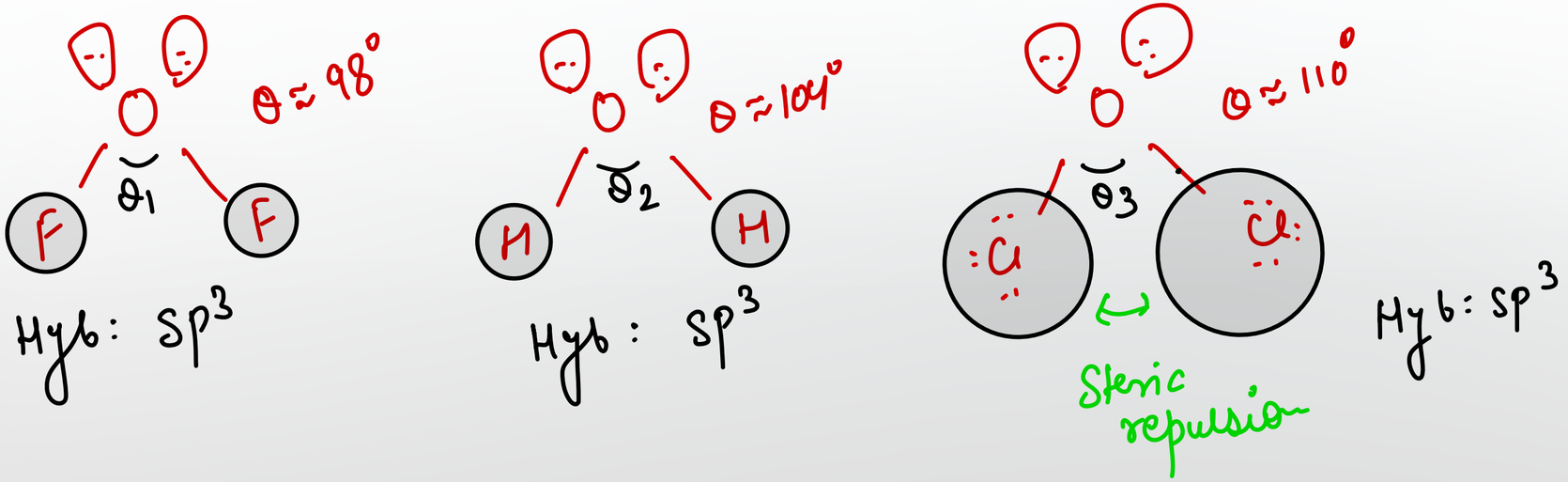
$\theta_2 > \theta_1$

Hybridization : sp^3

no of lone pair : 2 (Same)

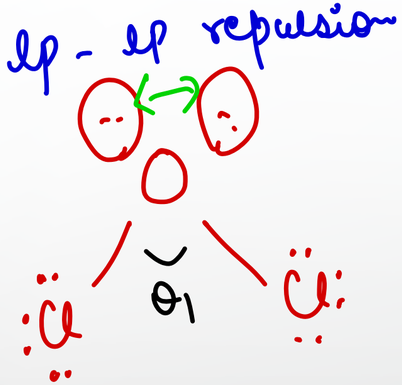
Central atom : Same

(Q) compare bond angle OF2 OH2 OCl2

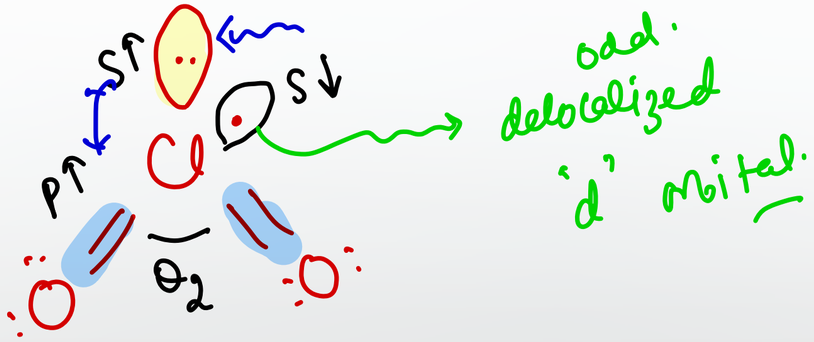


$\theta_3 > \theta_2 > \theta_1$

(Q) compare bond angle in OCl2 and ClO2



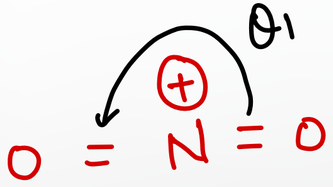
Hyb: sp^3



Hyb: sp^2

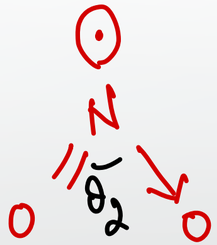
$\theta_2 > \theta_1$

(Q) compare bond angle between NO_2^+ NO_2 NO_2^-

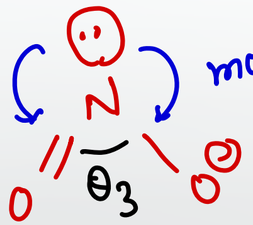


Hyb: sp

B.A : 180°



Hyb: sp^2

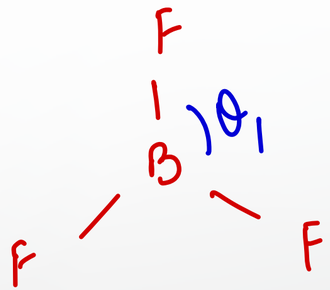


more repulsion compare to odder

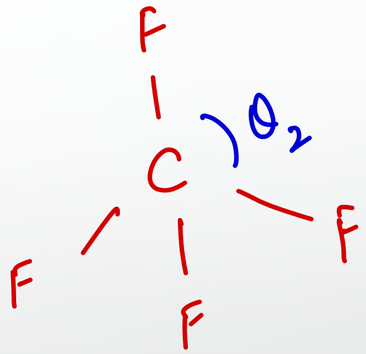
Hyb: sp^2

$\theta_1 > \theta_2 > \theta_3$

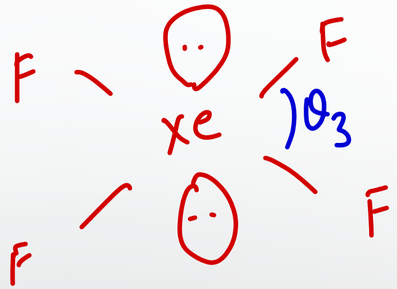
(Q) compare bond angle in BF3. CF4. XeF4



Hyb: sp^2



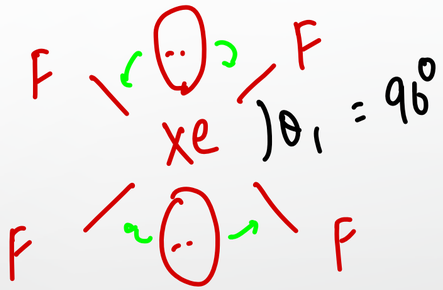
Hyb: sp^3

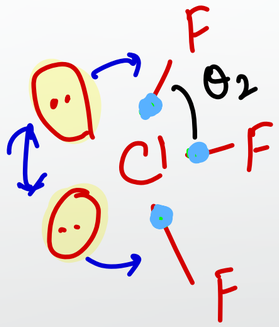


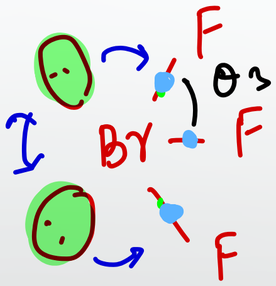
Hyb: sp^3d^2

$\theta_1 > \theta_2 > \theta_3$

Compare bond angle in XeF4. ClF3. BrF3

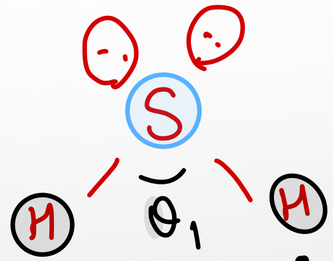






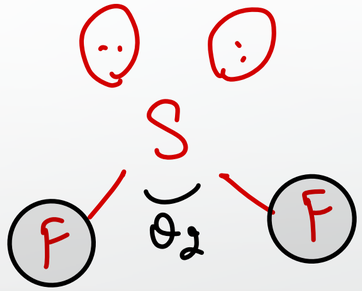
$$\{\theta_1 > \theta_2 > \theta_3\}$$

(Q) compare bond angle. H_2S. SF_2. SCl_2

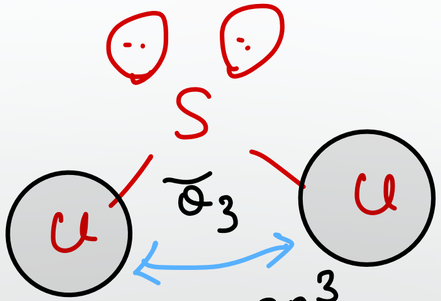


Drago's rule

$\theta_1 \simeq 92^0$



Hyb: sp^3

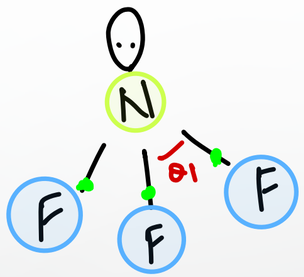


Hyb: sp^3

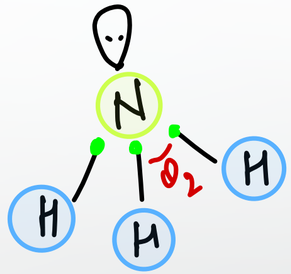
Size: steric repulsion

$\theta_3 > \theta_2 > \theta_1$

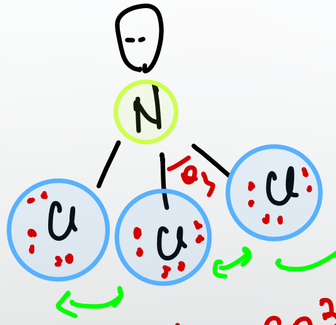
(Q) compare bond angle NF_3. NH_3. NCl_3



Hyb: sp^3



Hyb: sp^3



Steric repulsion

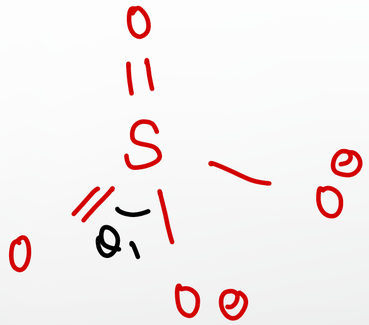
Hyb : sp^3

no of lone pair : Same

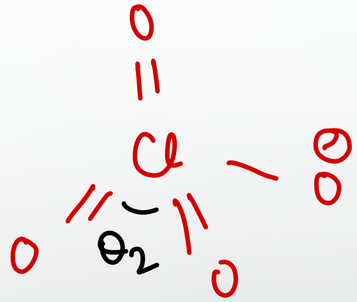
Central atom : Same.

$$\theta_3 > \theta_2 > \theta_1$$

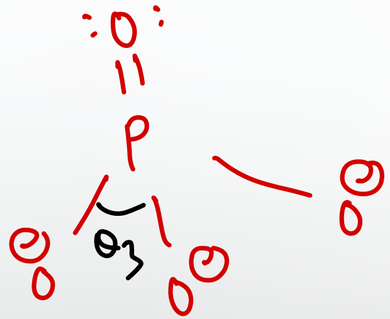
(Q) compare bond angle SO_4^{2-} ClO_4^- PO_4^{3-}



Hyb: sp^3



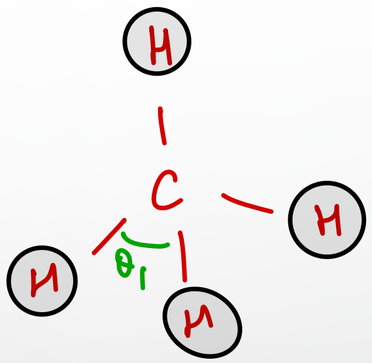
Hyb: sp^3



Hyb : sp^3

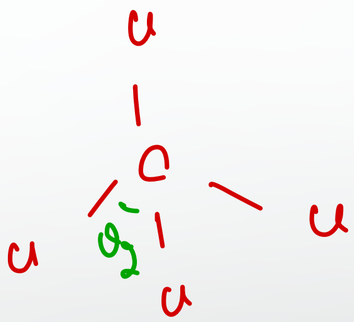
$\{\theta_1 = \theta_2 = \theta_3\}$

(Q) compare bond angle. CH_4. CCl_4. CF_4

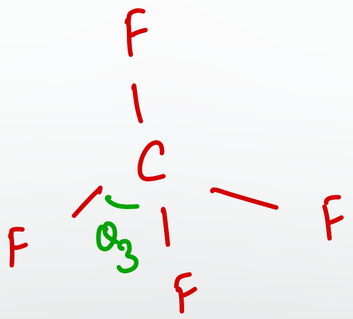


Hyb: sp^3

Geo: regular tetrahedral.



Hyb: sp^3



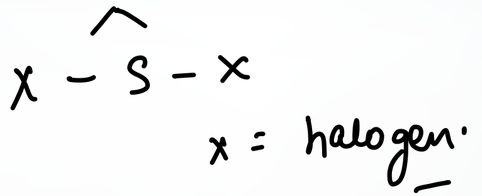
Hyb: sp^3

$\theta_1 = \theta_2 = \theta_3$

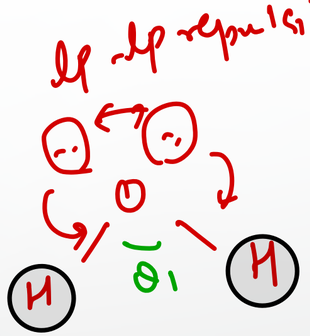
(Q) compare bond angle. BCl_3. $AlCl_3$. $GaCl_3$

$(\theta_1 = \theta_2 = \theta_3)$

H.W (Q) compare bond angle. SOF_2 < $SOCl_2$ < $SOBr_2$

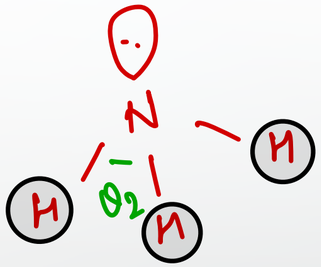


(Q) compare bond angle. H2O. NH3. N(CH3)3

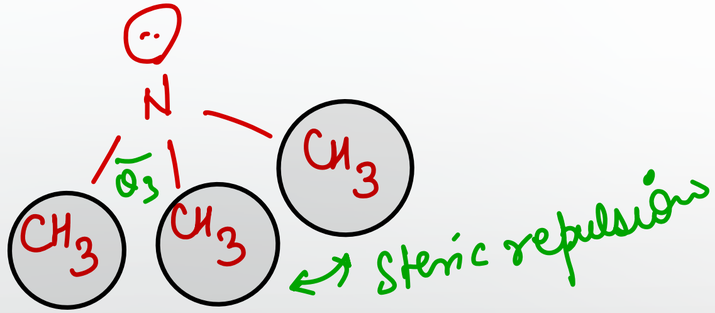


Hyb: sp^3

no of lone pair



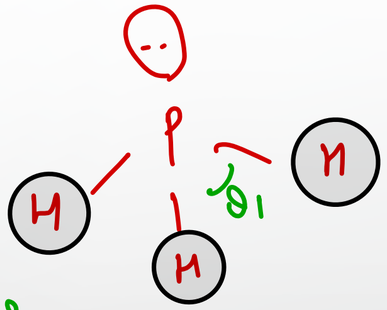
Hyb: sp^3



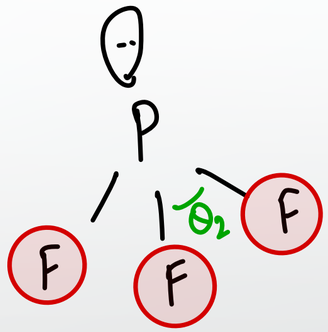
Hyb: sp^3

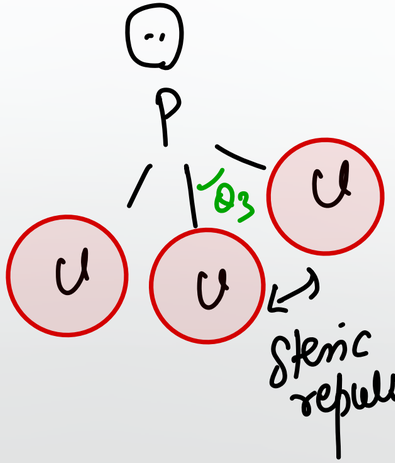
$\theta_3 > \theta_2 > \theta_1$

(Q) compare bond angle. PH_3. PF_3. PCl_3



Drago's Rule $\theta \simeq 92^\circ$





↳ repulsion due to large size of atom.

$$\theta_3 > \theta_2 > \theta_1$$

Bond length

Factors affecting bond length :

1. Size of atom
2. Bond order
3. Resonance

Comparison bond length

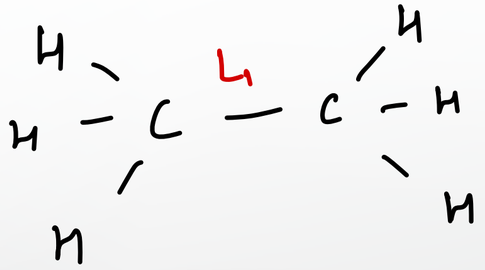
(a) $N \equiv N$ (b) $O = O$ (C) $F-F$

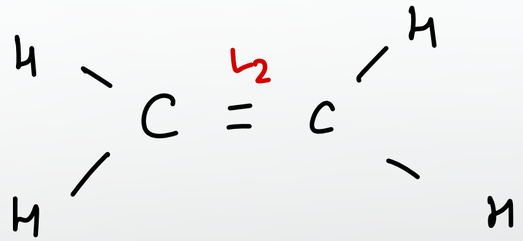
(B.O = 3.0) (B.O = 2.0) (B.O = 1.0)

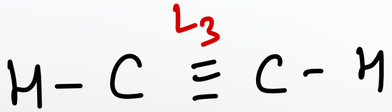
$$B.L \propto \frac{1}{B.O.}$$

(a) H_3C-CH_3 (b) $H_2C=CH_2$ (C) $HC\equiv CH$

Compare 'C - C' Bond length.







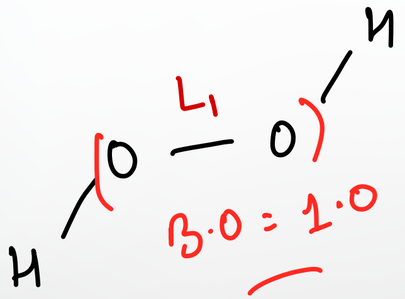
$L_1 > L_2 > L_3$.

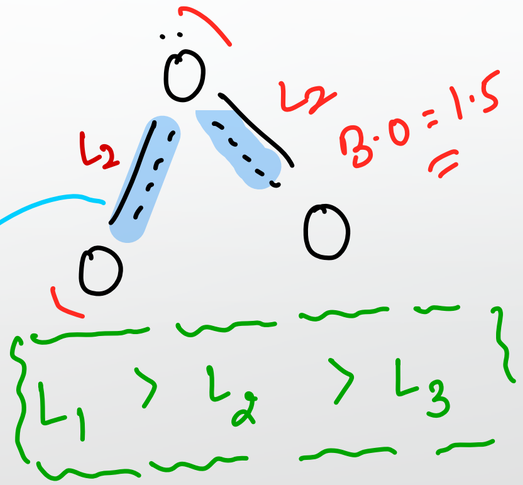
(c) HF HCl HBr HI

H - F < H - Cl < H - Br < H - I

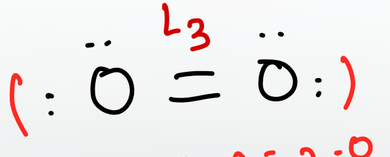
Comparism of B.L

(d) H_2O_2 O_3 O_2 Compare '$O-O$' Bond length.





partial double bond.



$\{L_1 > L_2 > L_3\}$

{* the Characteristic Bond length b/w double bond & Single bond}

{* Resonance}

(Q) compare bond length in (a) CO. CO2. CO_3^{2-}