Molecular Geometry

VSEPR model

- **Valence Shell Electron Pair Repulsion**
- **Shape of molecule is determined by the repulsion of electron pairs around the central atom.**
- **The repulsion must be minimum, i.e. Electron pairs are farthest from each other (potential energy minimum).**

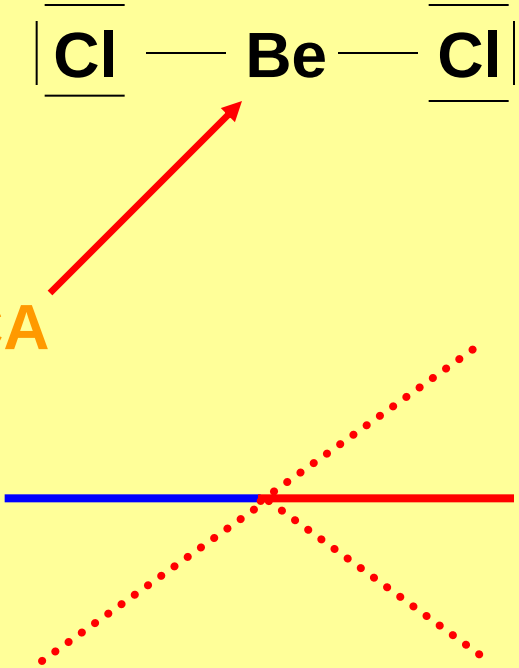
Rules

- *Draw the right Lewis Structure (formal charge!).*

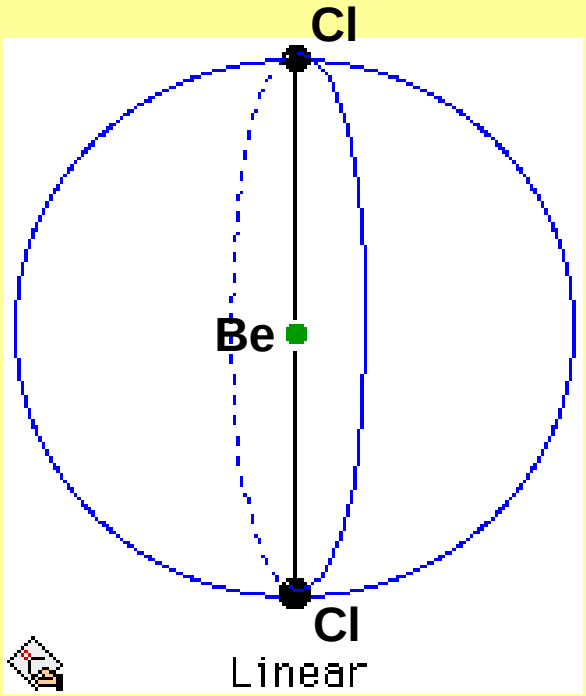
- *Determine the number of electron pairs around the central atom.*
  - ***Multiple bonds** are treated as if they were **one electron pair** because these electron pairs can not be separated from each other*
  - ***2, 3, 4, 5 or 6 EP.***

Two EP around Central Atom (AX_2)

$BeCl_2$



2 EP



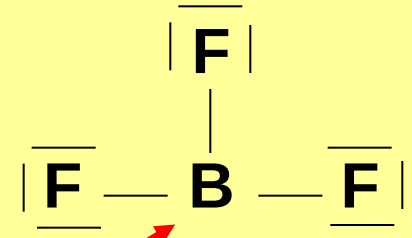
Shape: linear

Bond angle Cl-Be-Cl = 180°

X-A-X

Three EP around Central Atom (AX_3)

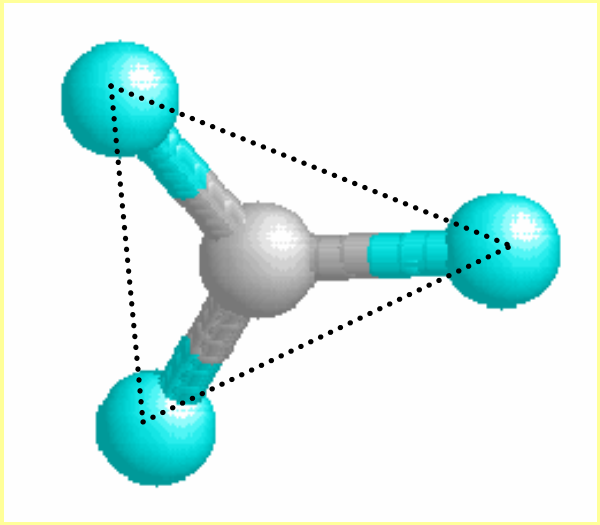
BF_3

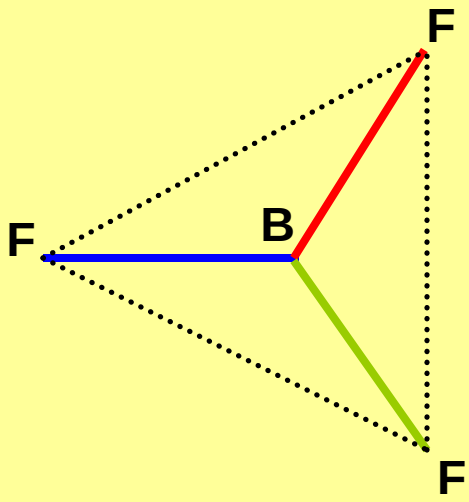


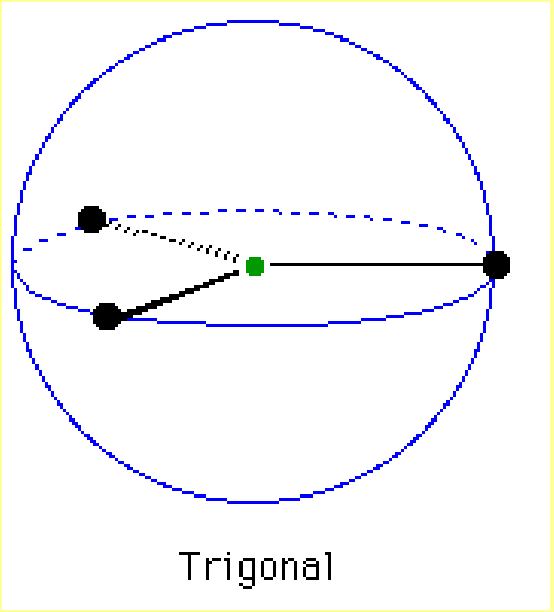
3 EP

AX_3

CA







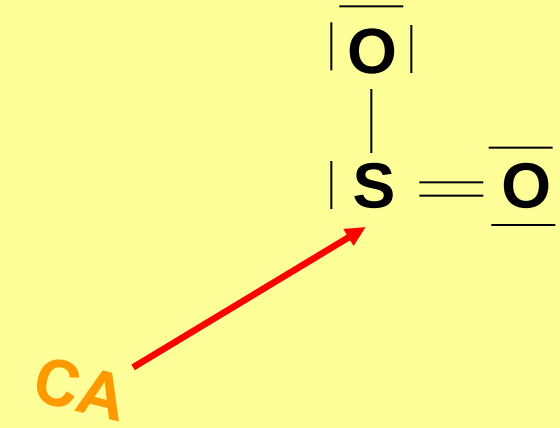
Shape: planar triangular

Bond angle F-B-F = 120º

X-A-X

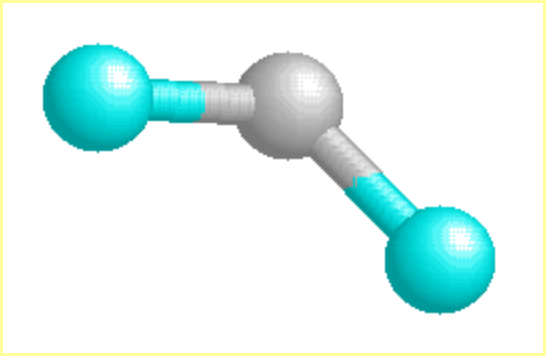
Three EP around Central Atom (AX_3)

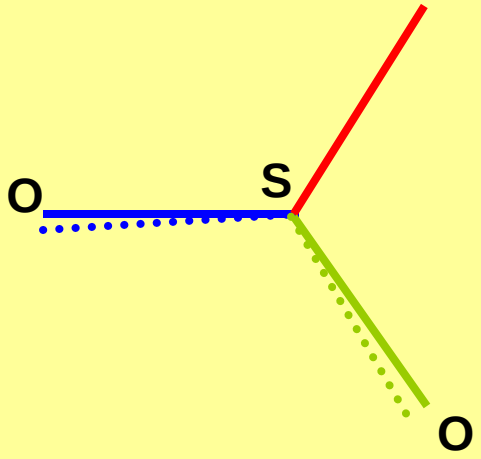
SO_2

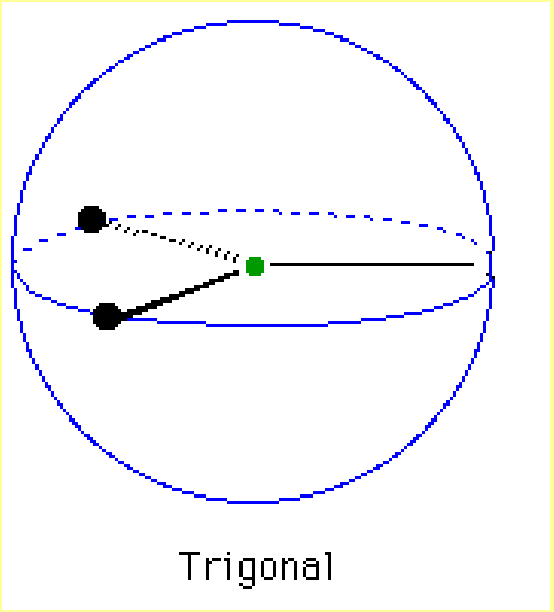


3 EP

AX_2E







Shape: *V-shaped (bent)*

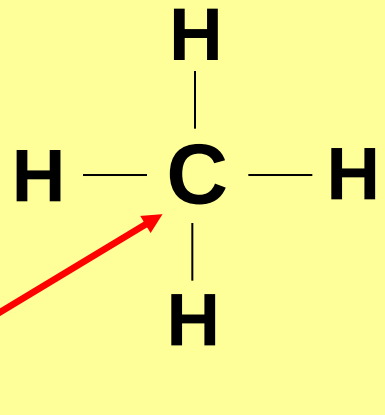
Bond angle *O-S-O* $\leq 120^o$

$\measuredangle$ *X-A-X*

Lone EP occupies a *larger space* than bonding EP.

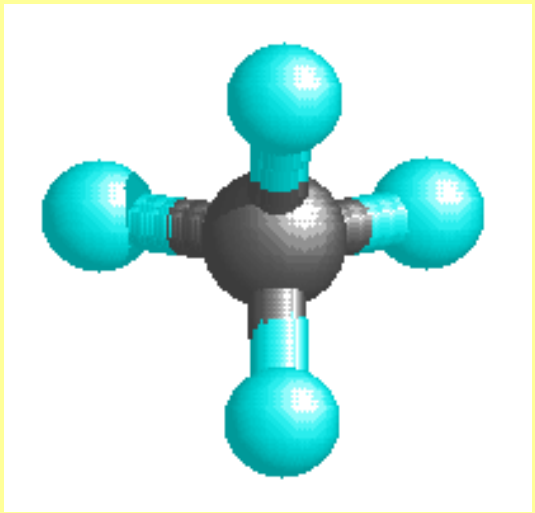
Four EP around Central Atom (AX_4)

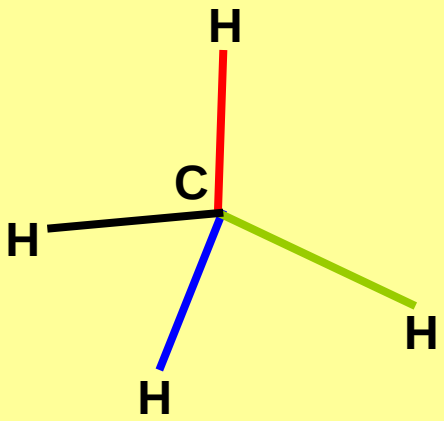
CH_4

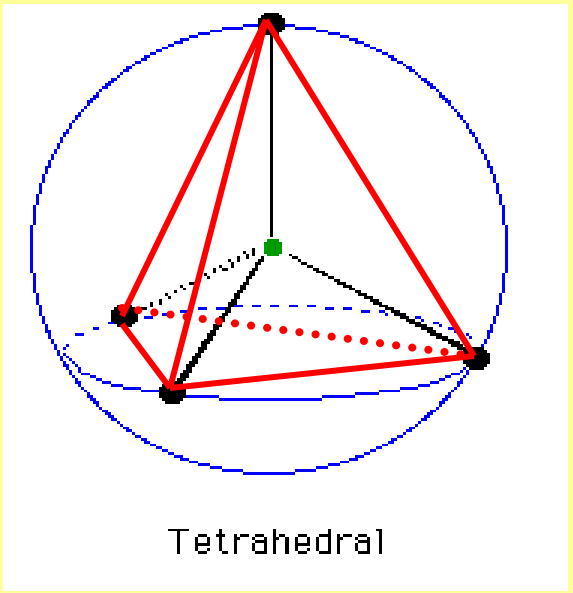


4 EP

AX_4







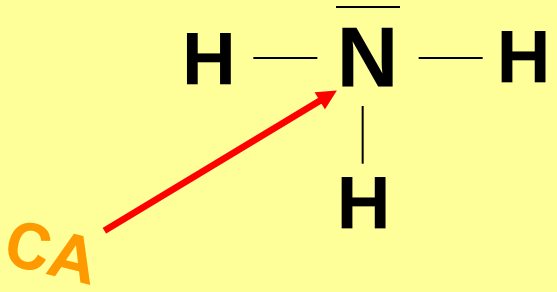
Shape: tetrahedral

Bond angle H-C-H = 109.5°

X-A-X

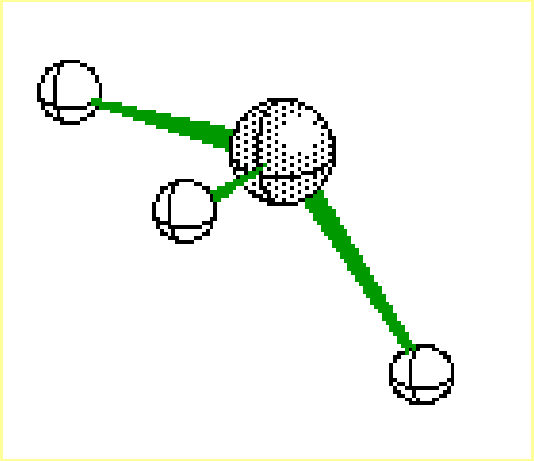
Four EP around Central Atom (AX_4)

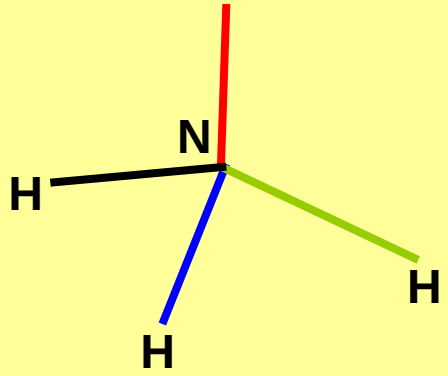
NH_3

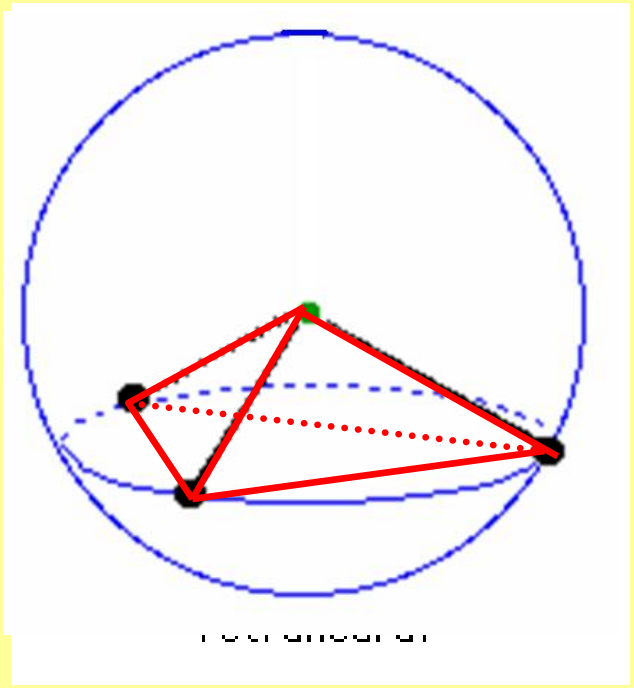


4 EP

AX_3E







Shape:* *trigonal pyramidal

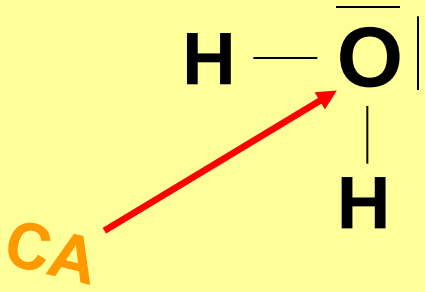
Bond angle* *H-N-H* $\prec$ *109.5°

$\hookleftarrow$ *X-A-X*

Lone EP occupies a *larger space* than bonding EP.

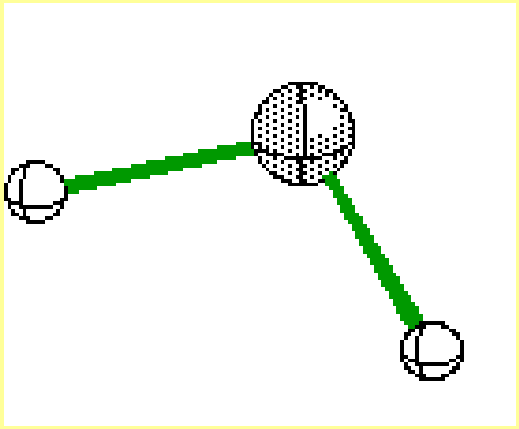
Four EP around Central Atom (AX_4)

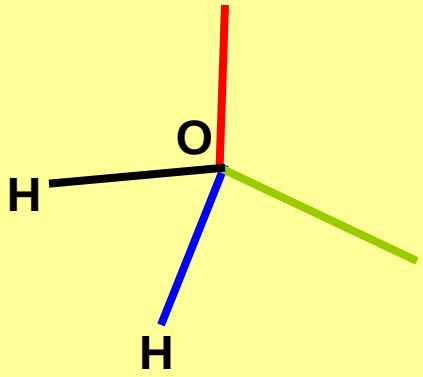
H_2O

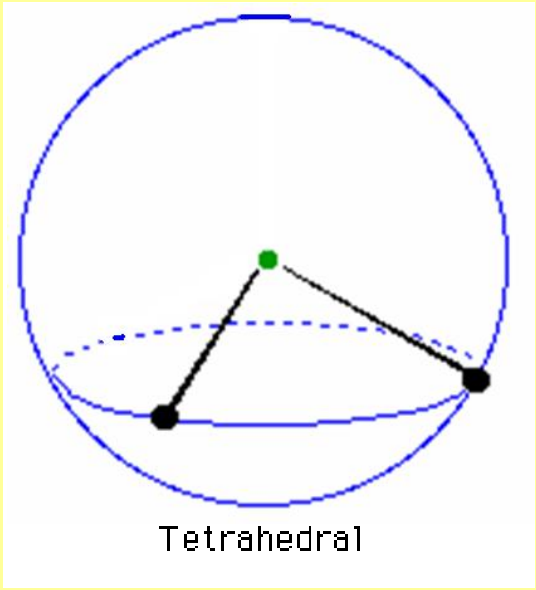


4 EP

AX_2E_2







Shape:* *V-shaped

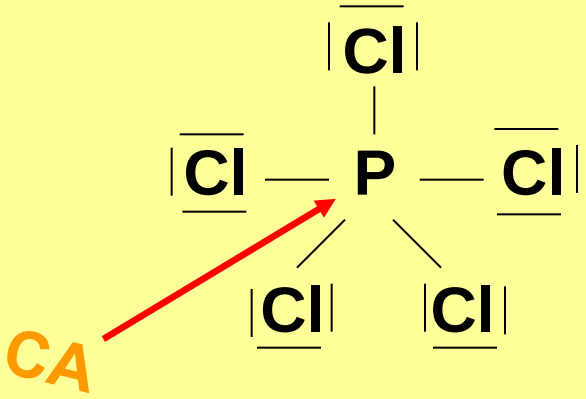
Bond angle* *H-O-H* $<$ *109.5°

$<$ *X-A-X*

Lone EP occupies a *larger space* than bonding EP.

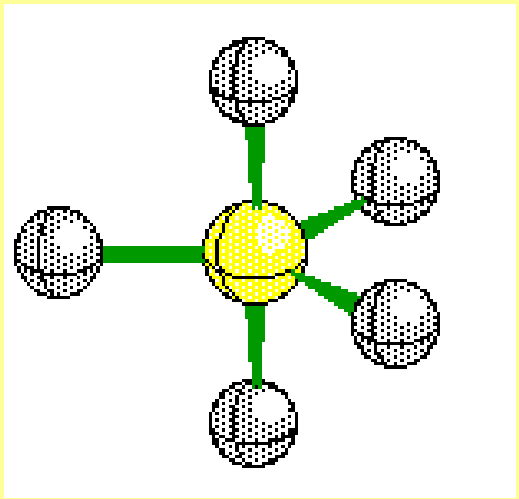
Five EP around Central Atom (AX_5)

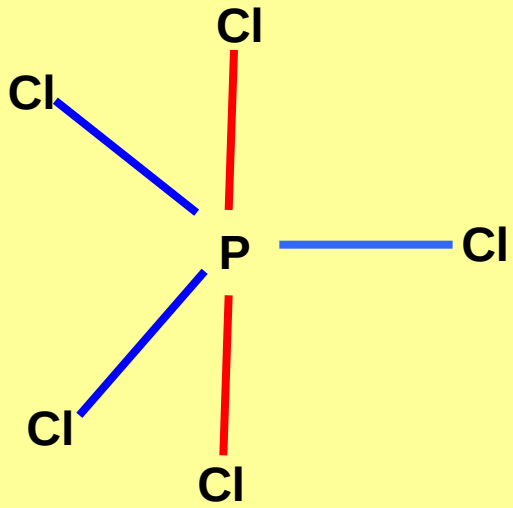
PCl_5

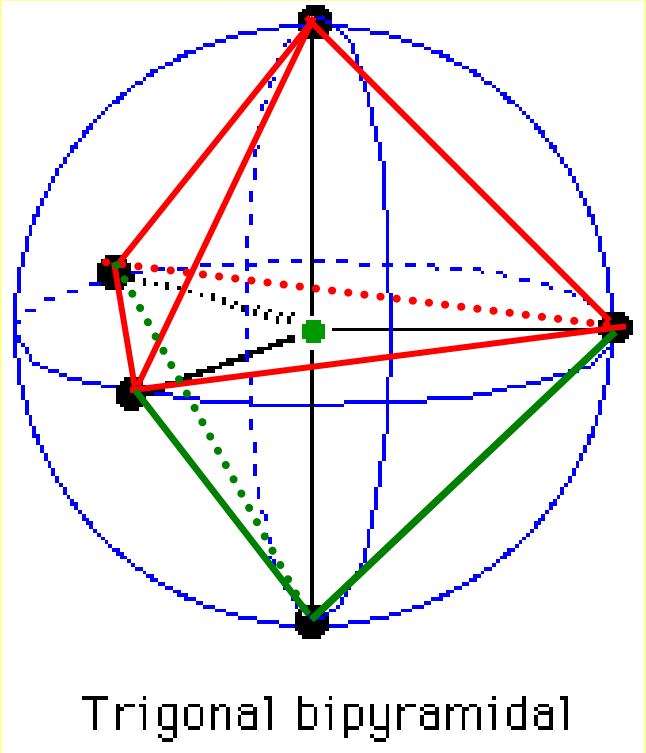


5 EP

AX_5







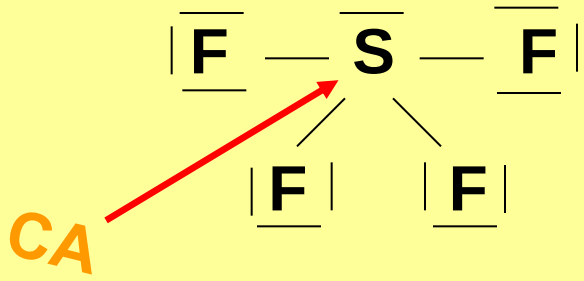
Shape: trigonal bipyramidal

Bond angle Cl-P-Cl = 120º, 90º

X-A-X

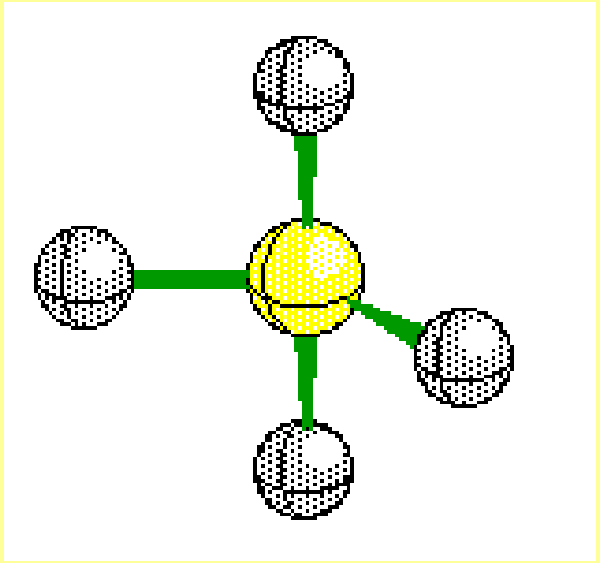
Five EP around Central Atom (AX_5)

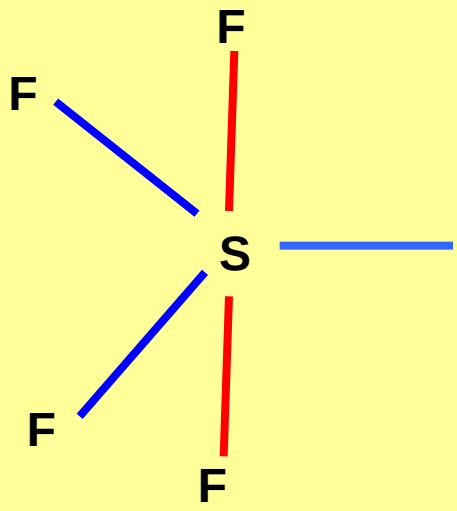
SF_4

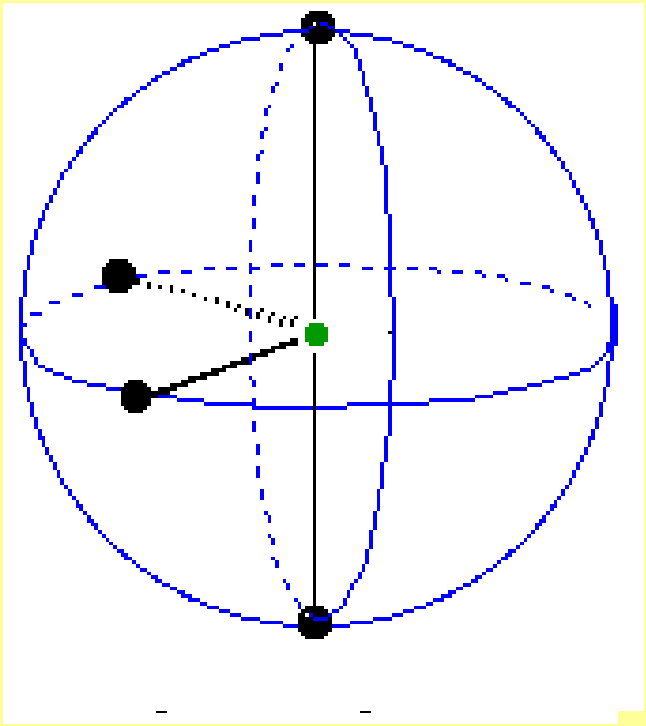


5 EP

AX_4E







Lone EP occupies a ***larger space*** than bonding EP.

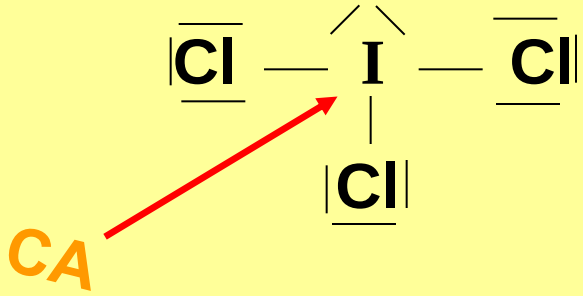
Shape: *disordered tetrahedral*

Bond angle *Cl-P-Cl = 120º, 90º*

X-A-X

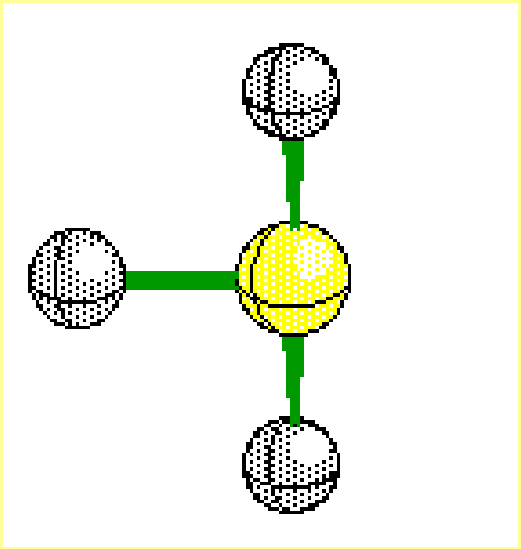
Five EP around Central Atom (AX_5)

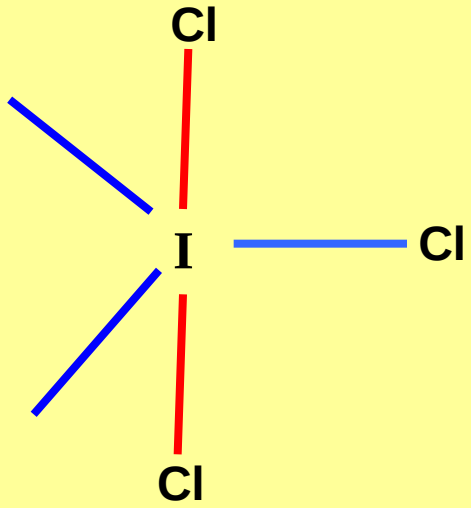
ICl_3

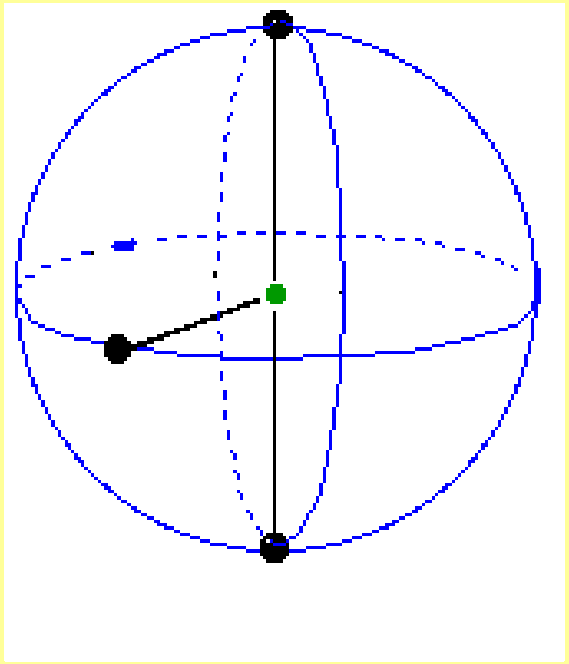


5 EP

AX_3E_2







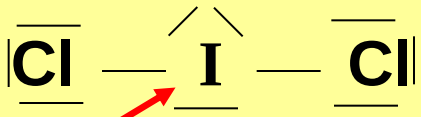
Lone EP occupies a ***larger space*** than bonding EP.

Shape: T-shaped

Bond angle Cl-P-Cl = 120º, 90º

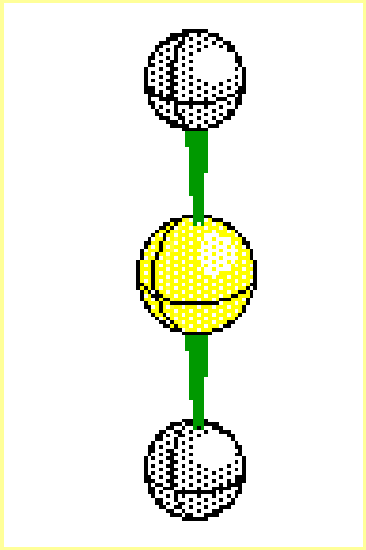
X-A-X

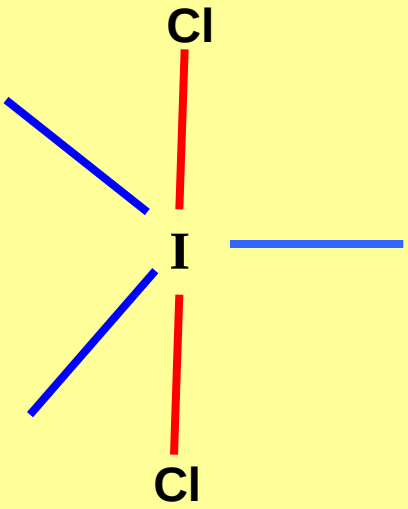
Five EP around Central Atom (AX_5)

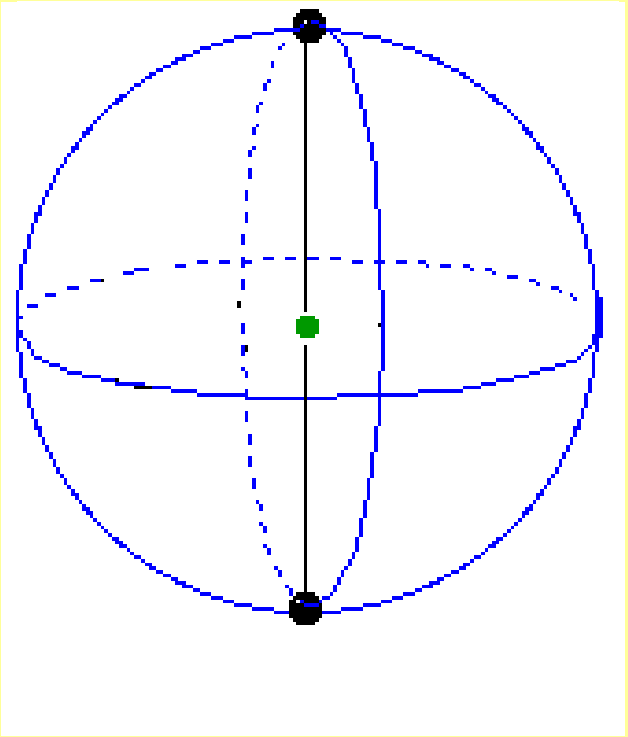
ICl_2^- 

5 EP AX_2E_3

CA







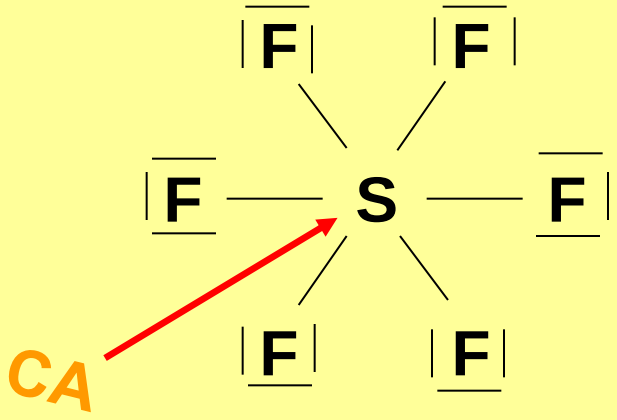
Lone EP occupies a ***larger space*** than bonding EP.

Shape: linear ***Bond angle Cl-I-Cl = 180°***

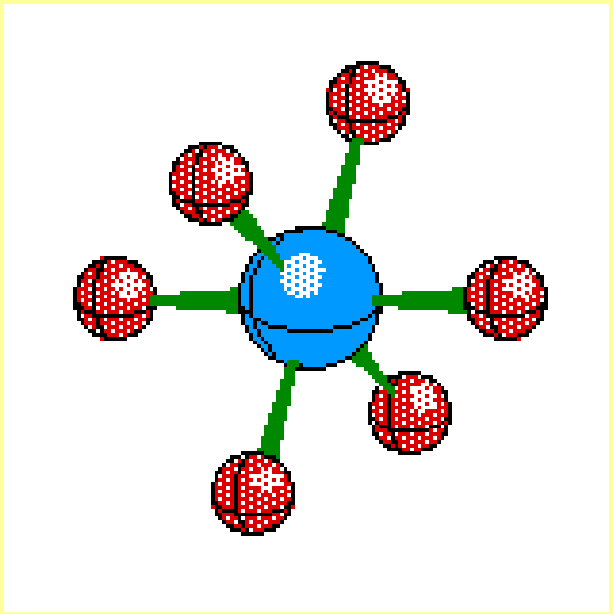
X-A-X

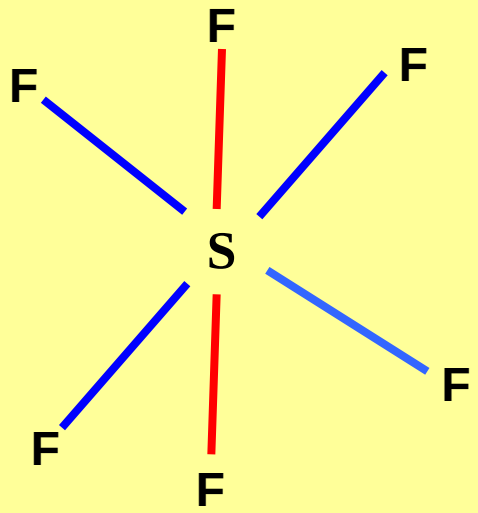
Six EP around Central Atom (AX_6)

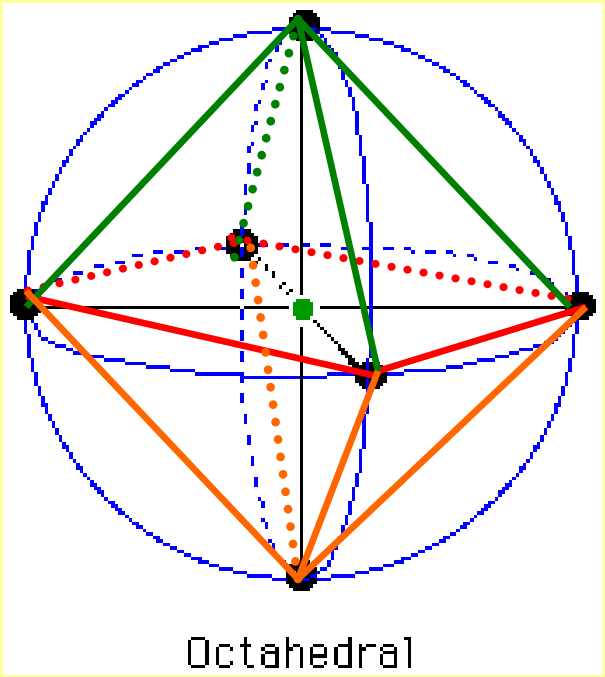
SF_6



6 EP AX_6







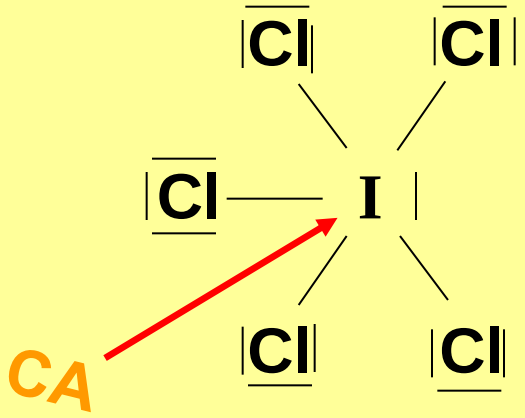
Shape: octahedral

Bond angle F-S-F = 90°

X-A-X

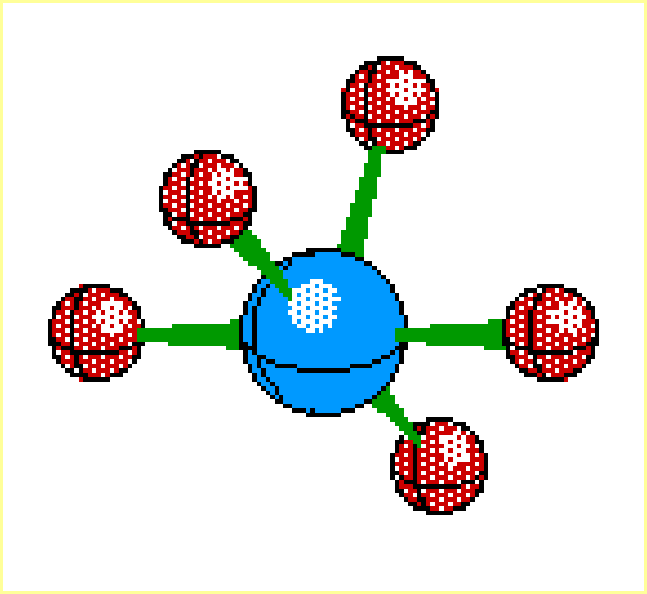
Six EP around Central Atom (AX_6)

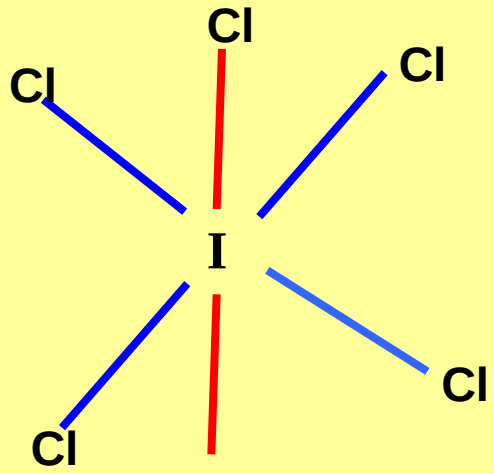
ICl_5

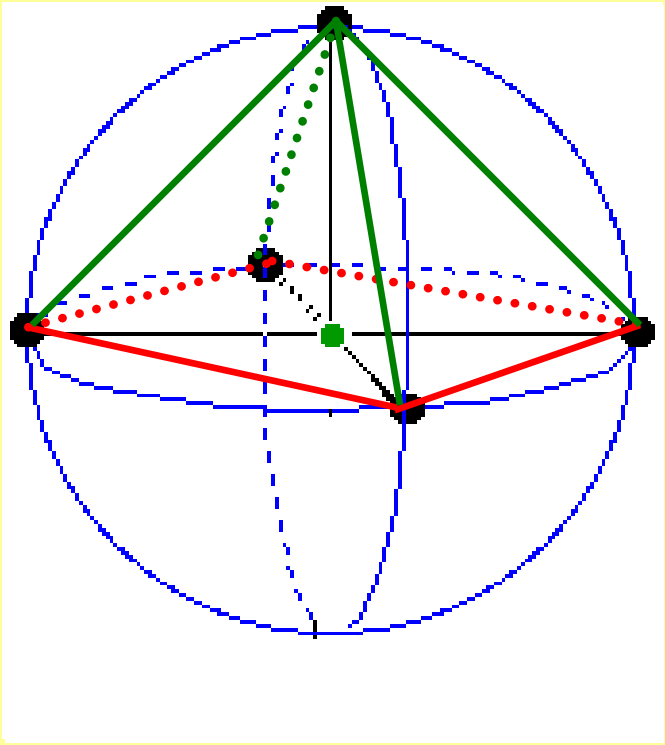


6 EP

AX_5E







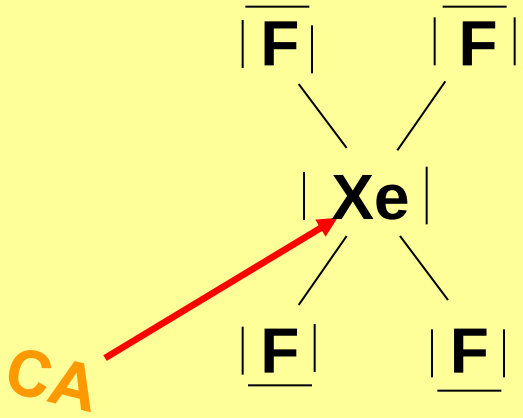
Shape: square pyramidal

Bond angle Cl-I-Cl = 90°

X-A-X

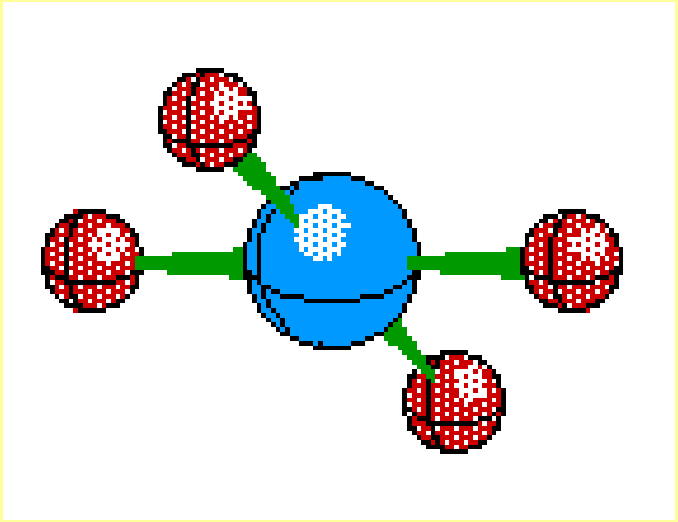
Six EP around Central Atom (AX_6)

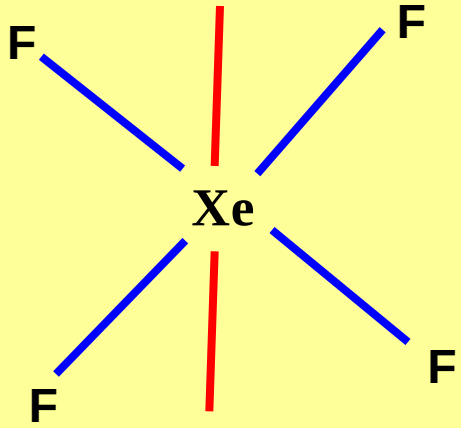
XeF_4

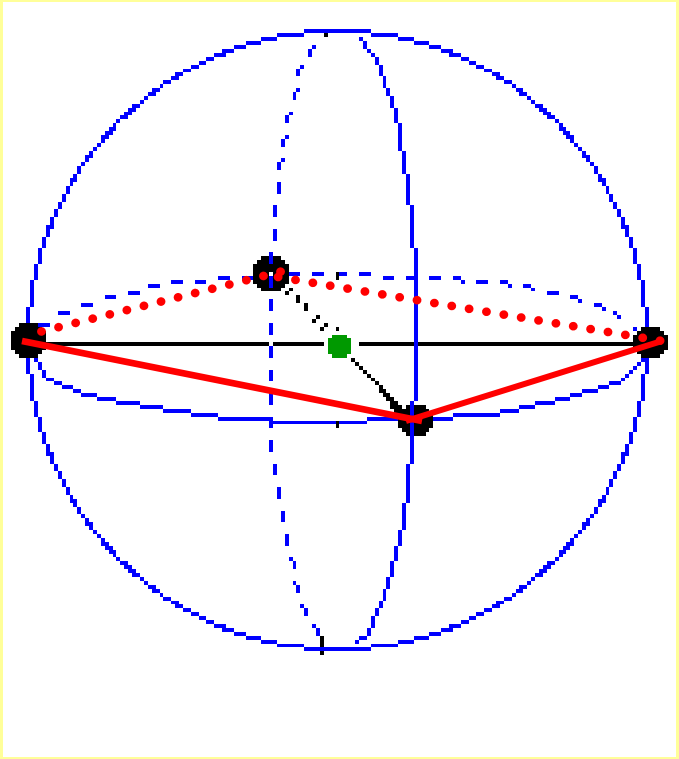


6 EP

AX_4E_2







Shape: square planar

Bond angle F-Xe-F= 90°

X-A-X

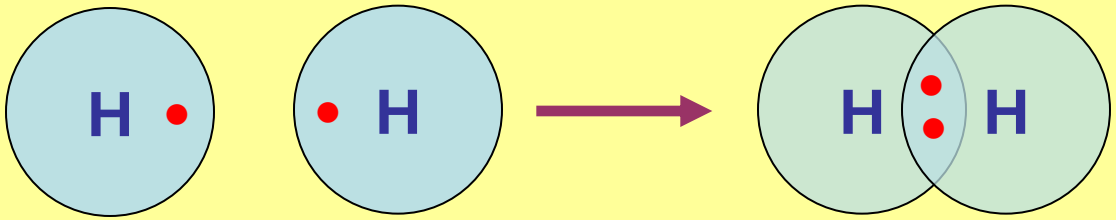
Group	Type	Example	Molecular Geometry	polarity	Bond angle
2	AX_2	$BeCl_2$	linear	×	180º
3	AX_3	BF_3	planar triangular	×	120º
	AX_2E	SO_2	V-shaped	✓	<120º
4	AX_4	CH_4	tetrahedral	×	109.5º
	AX_3E	NH_3	trigonal pyramidal	✓	<109.5º
	AX_2E_2	H_2O	V-shaped	✓	<109.5º
5	AX_5	PCl_5	trigonal bipyramidal	×	120º, 90º
	AX_4E	SF_4	disordered tetrahedral	✓	120º, 90º
	AX_3E_2	ICl_3	T-shaped	✓	90º
	AX_2E_3	ICl_2^-	linear	×	180º
6	AX_6	SF_6	octahedral	×	90º
	AX_5E	ICl_5	square pyramidal	✓	90º
	AX_4E_2	XeF_4	square planar	×	90º

Hybridization

How is the bond formed in H_2 molecule?

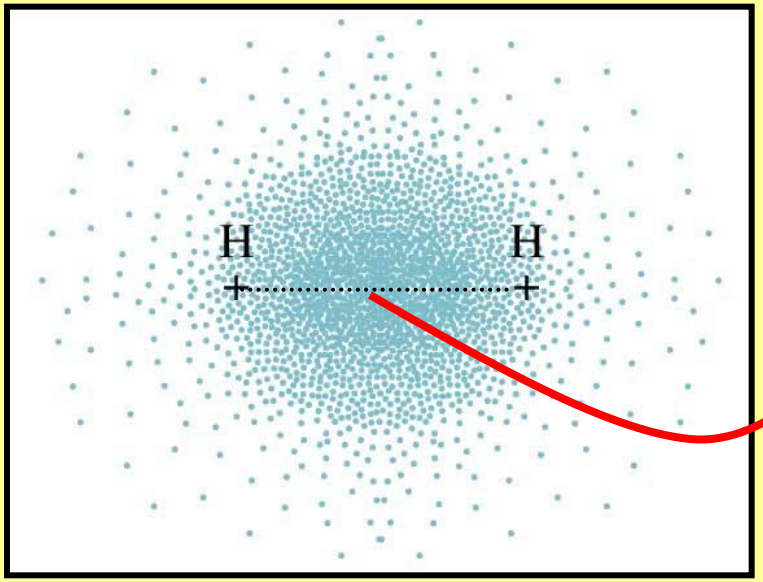
H• + •H ⟶ H-H

1s



1s *1s*

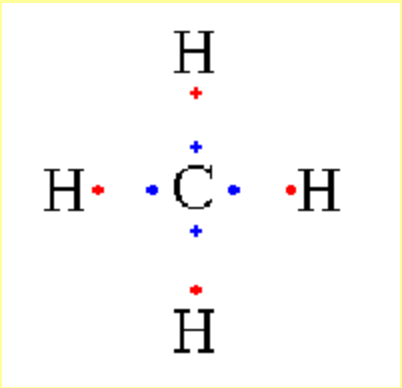
Overlap of $1s_H$-$1s_H$

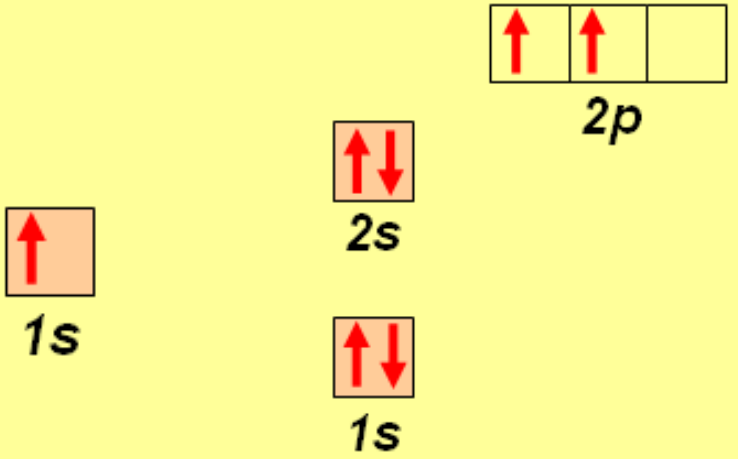


Increase in the electron density on the line connecting the two nuclei.

⇨ **σ-bond**

How is the bond formed in CH_4 molecule?



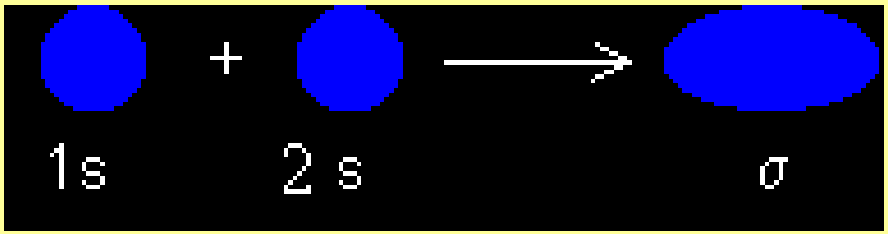


Problem: *Only two unpaired electrons in C atom!! CH_2!!!!*

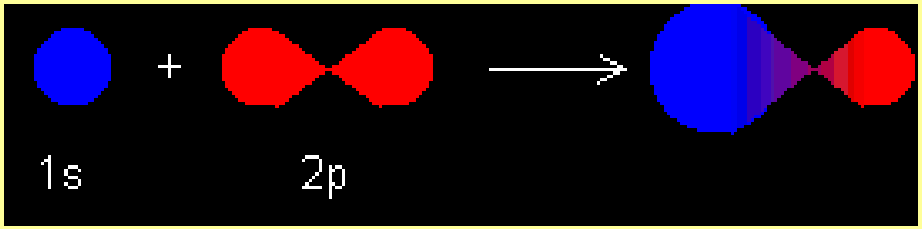
Now: *4 unpaired electrons in C atom ⇨ 4 bonds!*

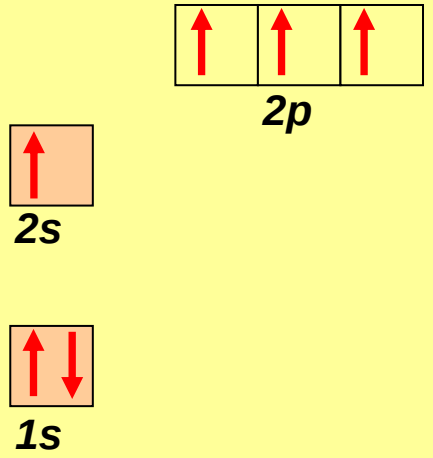
Problem: *bonds are not equivalent:*

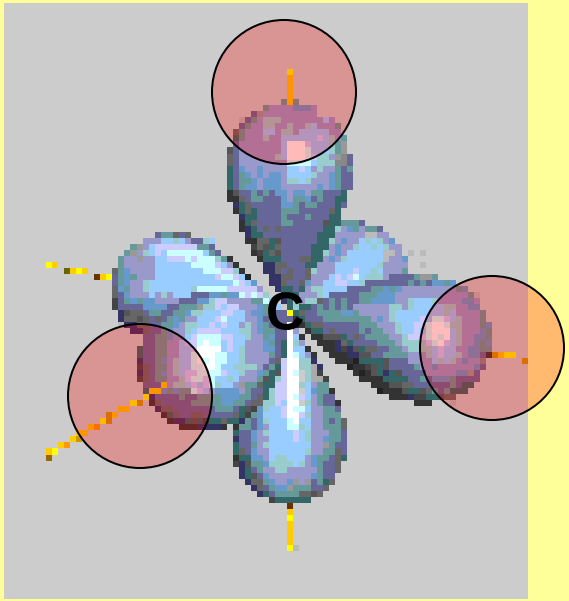
1 bond



3 bonds



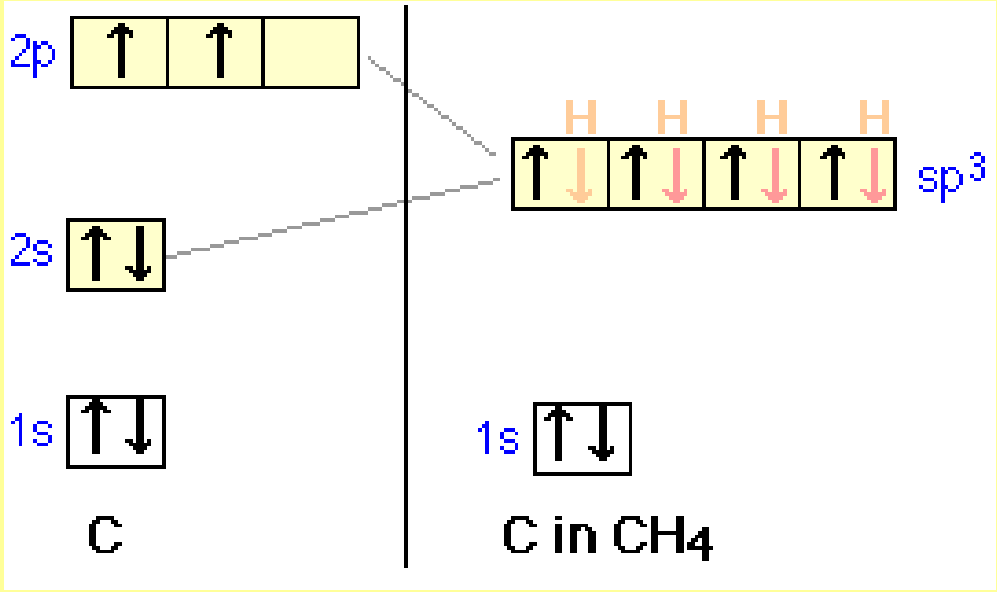




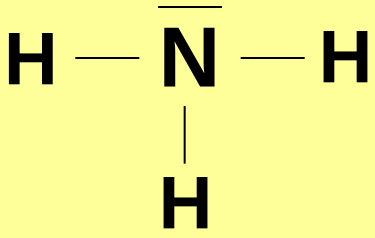
Bond angle H-C-H = 90° NOT 109.5°

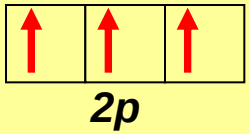
can not be correct!

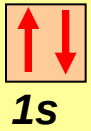
Hybridization



How is the bond formed in NH_3 molecule?



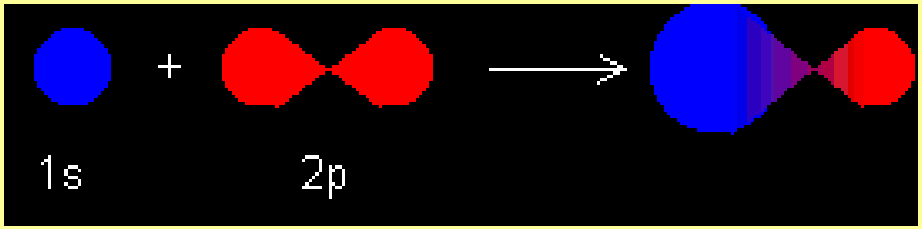


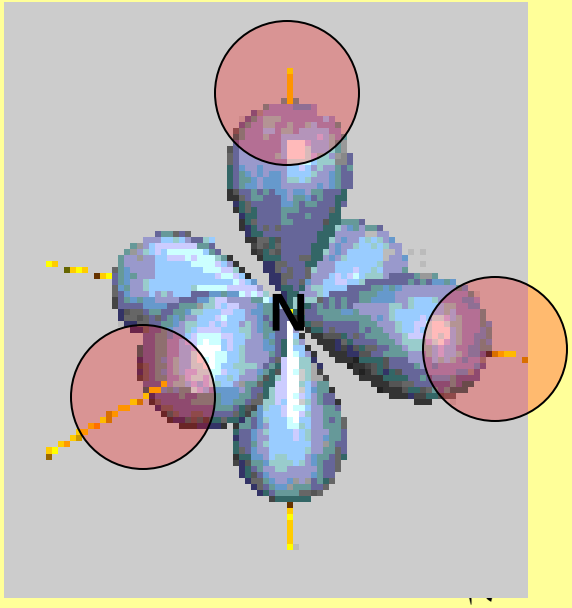


Overlap of $1s_H$-$2p_N$??

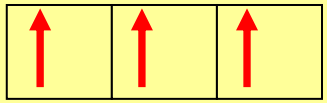
Problem: *bonds are perpendicular to each other!!*

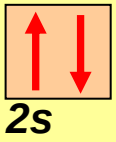
3 bonds

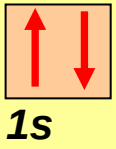


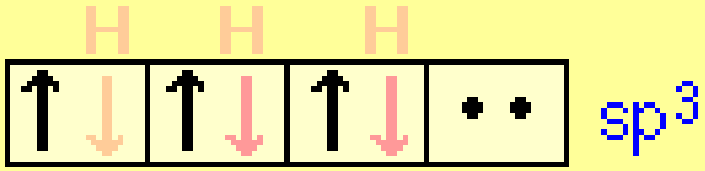


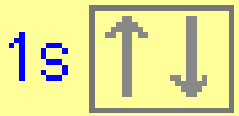
Actually 107º which is close to 109.5 º not to 90 º.





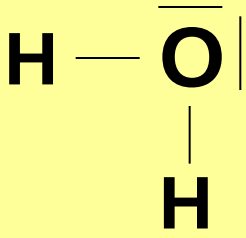


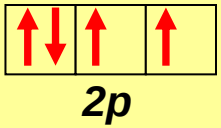


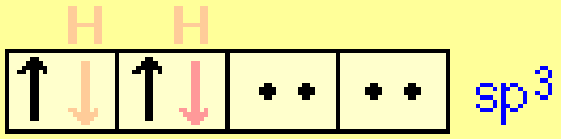


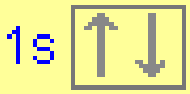
N in NH_3

Overlap of s_H-$sp^3{}_N$



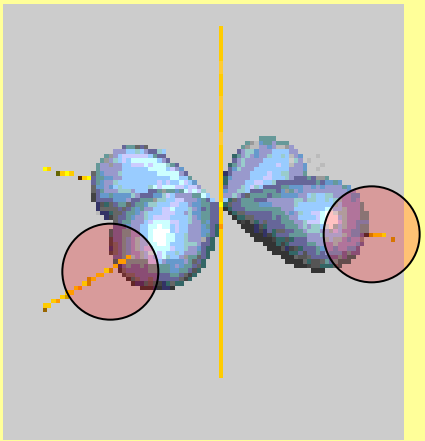


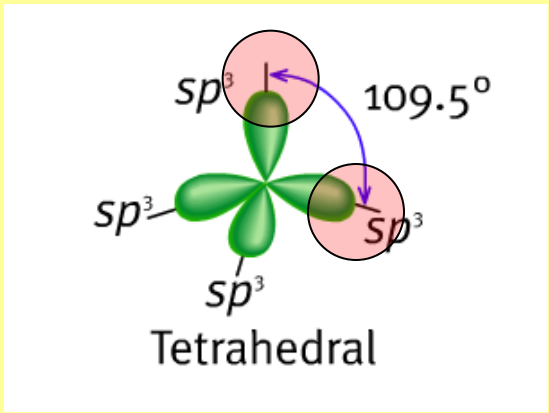




O in H_2O

Bond angle 90º!!





No. of mixed orbitals =
No. of σ bonds + No. of lone EP

CH_4: 4+0 = 4 (1 s + 3 p) = 4 sp^3

NH_3: 3+1 = 4 (1 s + 3 p) = 4 sp^3

H_2O: 2+2 = 4 (1 s + 3 p) = 4 sp^3

Key number

No. of mixed orbitals = No. of σ bonds + No. of lone EP

Key number	*Hybridi-zation*	*Group*	*Type*	*Molecular Geometry*
2	*sp*	*2*	*AX_2*	*linear*
3	*sp^2*	*3*	*AX_3*	*planar triangular*
			AX_2E	*V-shaped*
4	*sp^3*	*4*	*AX_4*	*tetrahedral*
			AX_3E	*trigonal pyramidal*
			AX_2E_2	*V-shaped*
5	*sp^3d*	*5*	*AX_5*	*trigonal bipyramidal*
			AX_4E	*disordered tetrahedral*
			AX_3E_2	*T-shaped*
			AX_2E_3	*linear*
6	*sp^3d^2*	*6*	*AX_6*	*octahedral*
			AX_5E	*square pyramidal*
			AX_4E_2	*square planar*