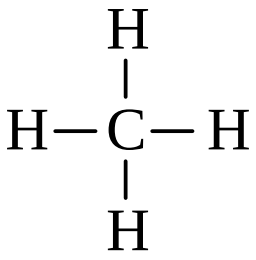
Molecular Shapes

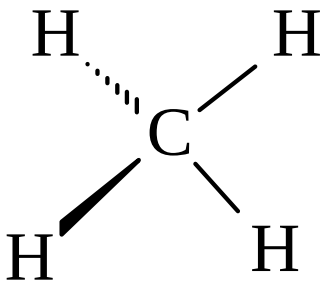
CH_4



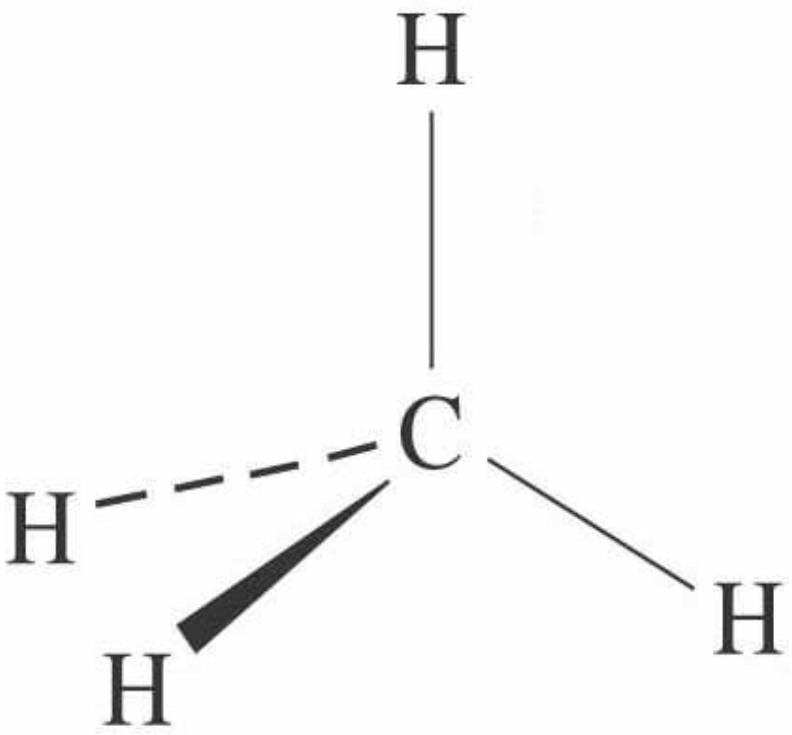
flat (planar)?

90^o and 180^o angles?

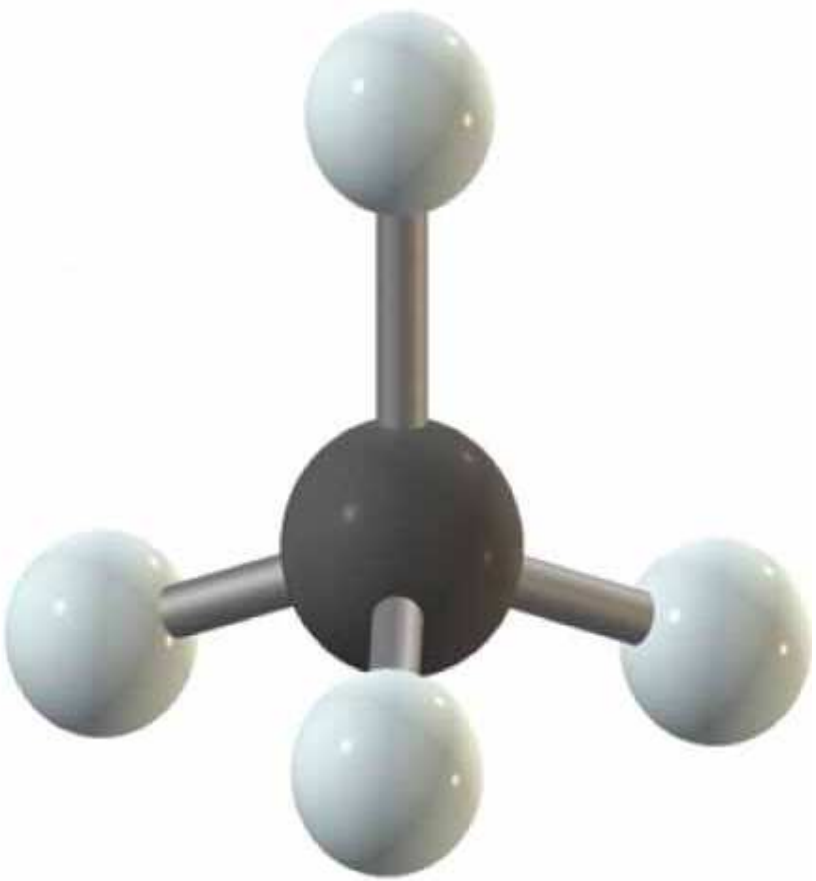
the shape is 3 dimensional



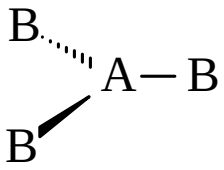
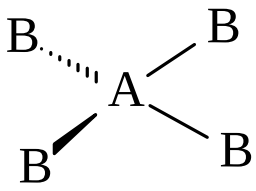
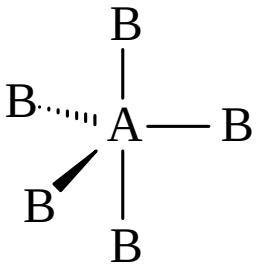
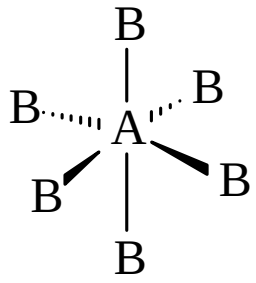
A Model



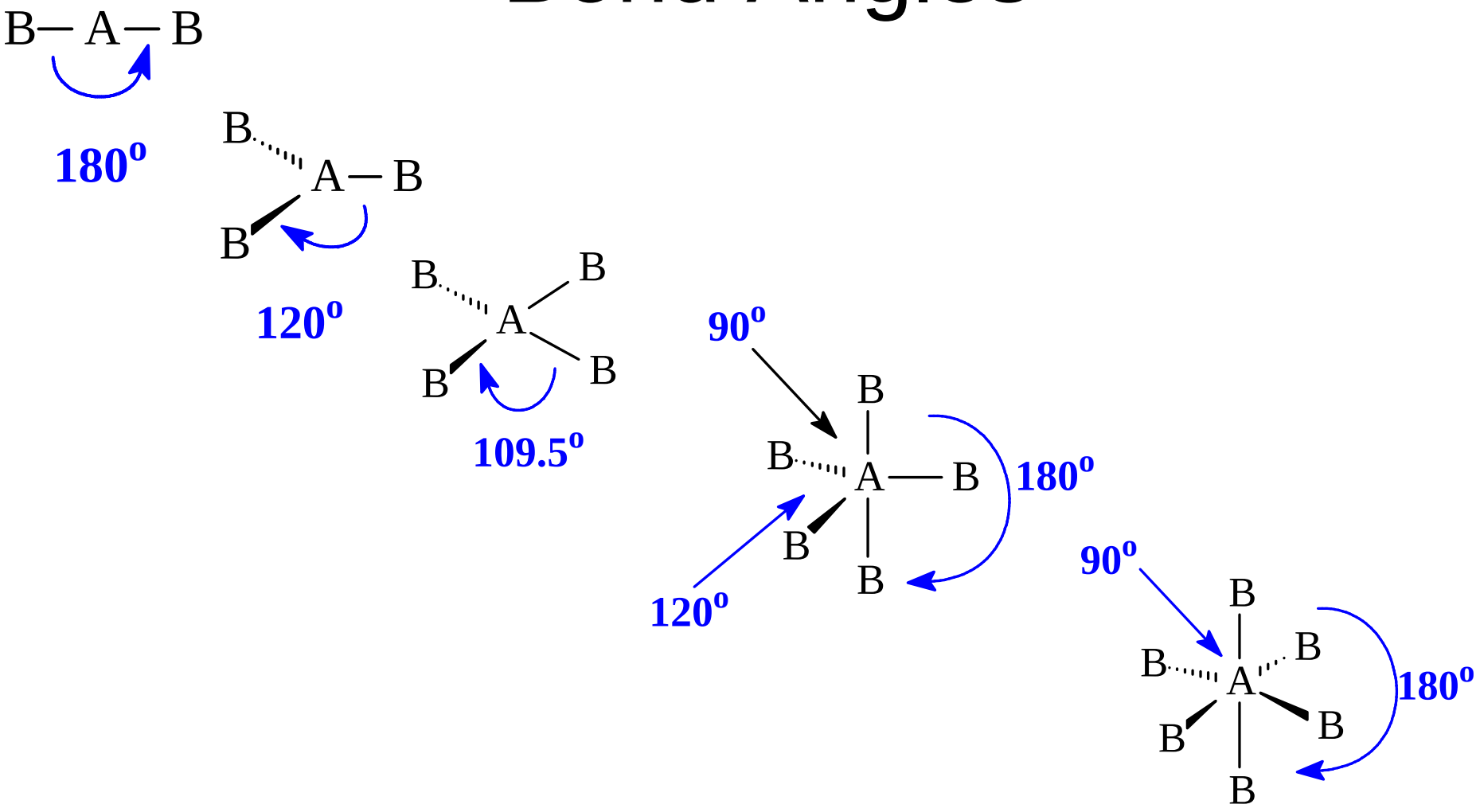
CH_4



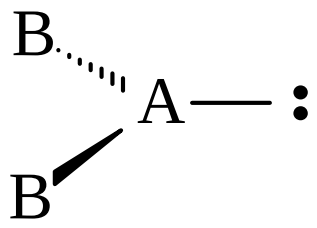
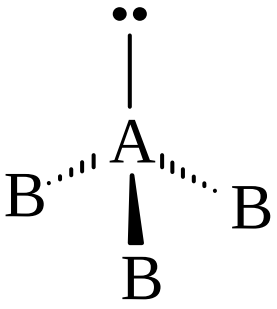
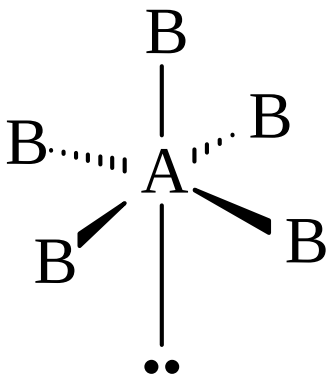
Shapes Based on Number of Surrounding Atoms

	AB_2	AB_3	AB_4	AB_5	AB_6
count	**2**	**3**	**4**	**5**	**6**
	B─ A─ B				
	linear	trigonal planar	tetrahedral	trigonal bipyramid(al)	octahedral

Bond Angles

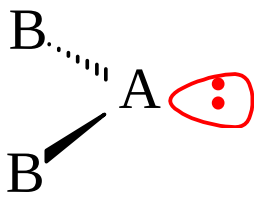


Lone Pairs Count!

$\ddot{A}B_2$	$\ddot{A}B_3$	$\ddot{A}B_4$	$\ddot{A}B_5$
3	**4**	**5**	**6**
		**?**	
trigonal planar	tetrahedral	trigonal bipyramid(al)	octahedral

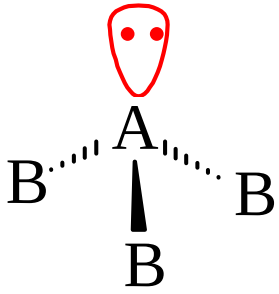
Lone Pairs Cannot be Seen

3



bent
(angular)

4

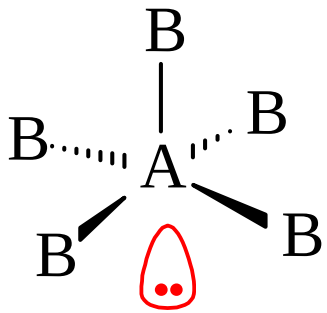


trigonal
pyramid(al)

5

?

6



square
pyramid(al)

2 Sets of Lone Pairs

4	5	6
$:\ddot{A}B_2$	$:\ddot{A}B_3$	$:\ddot{A}B_4$
	?	?

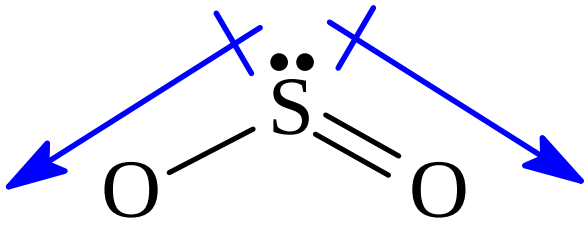
An Application

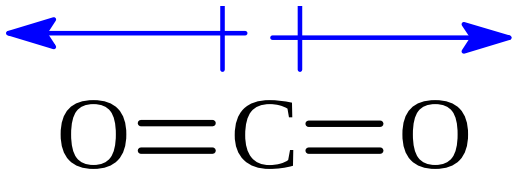
SO_2 vs CO_2

S and C have almost identical electronegativities
therefore the C-O and S-O bond are equally polar

But CO_2 is non-polar and SO_2 is polar

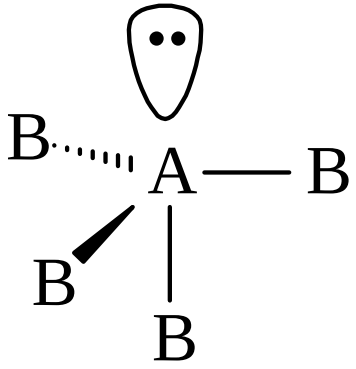
Dipoles are Vectors

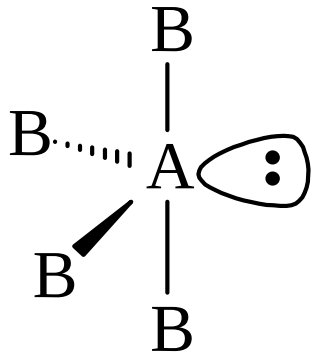




Back to :AB_4

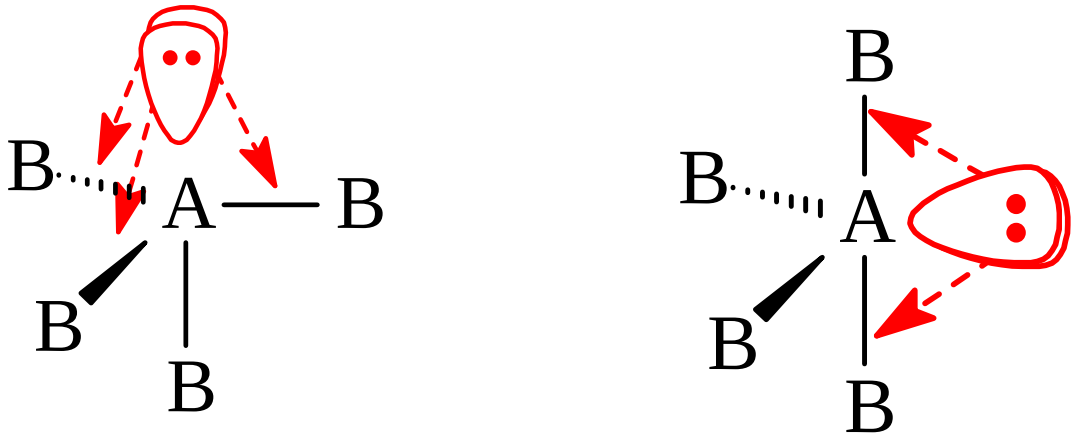
different structures





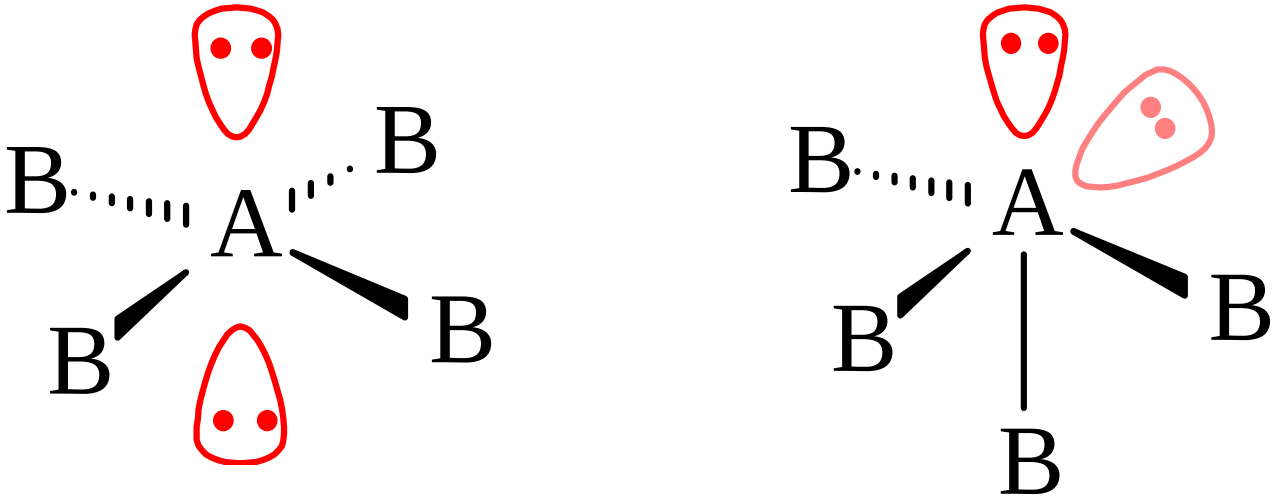
select the better one by considering **lone pair-bond pair** interactions

LP-BP Interactions



Lone Pair-Lone Pair Interactions (the worst kind of repulsive interaction)

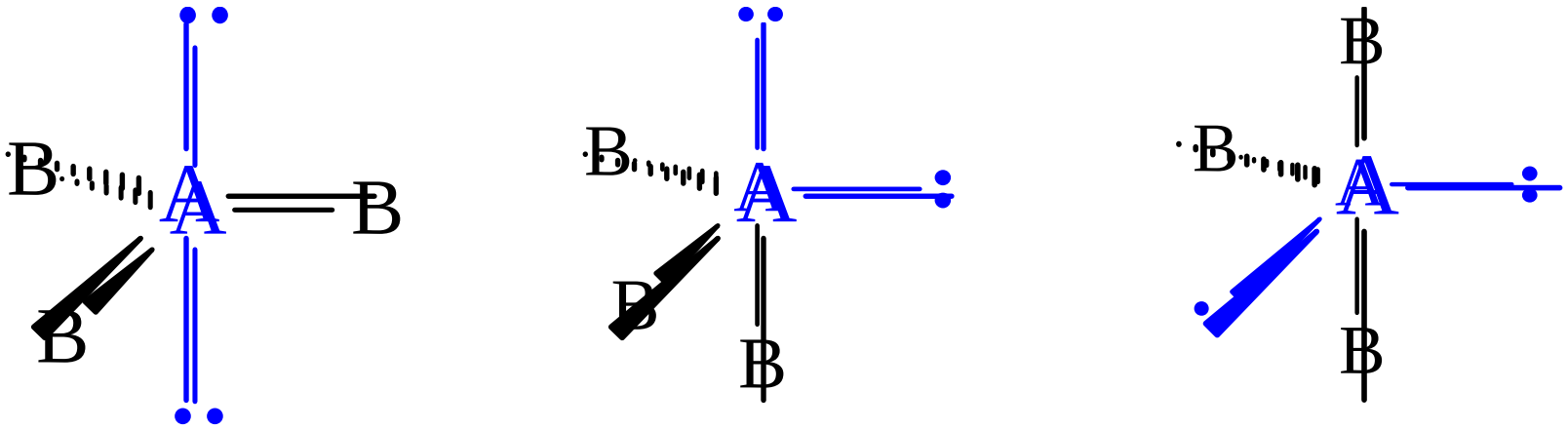
$:\ddot{A}B_4$



Another Example

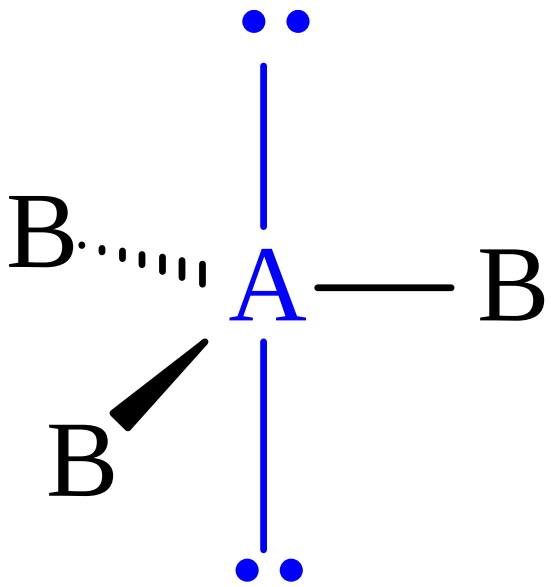
$:\ddot{A}B_3$

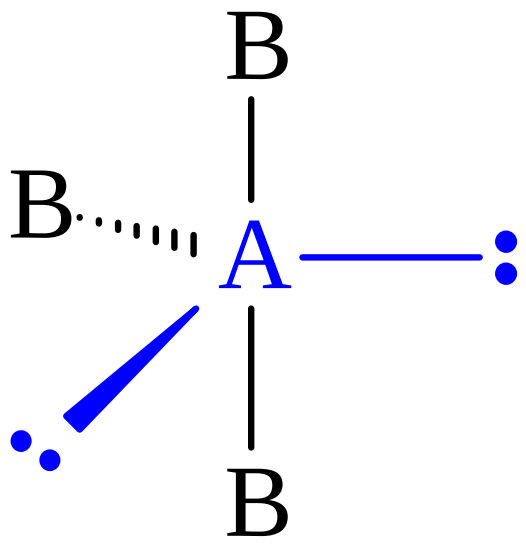
(hint: how many bond angles are there?)



assign LP-LP to all structures

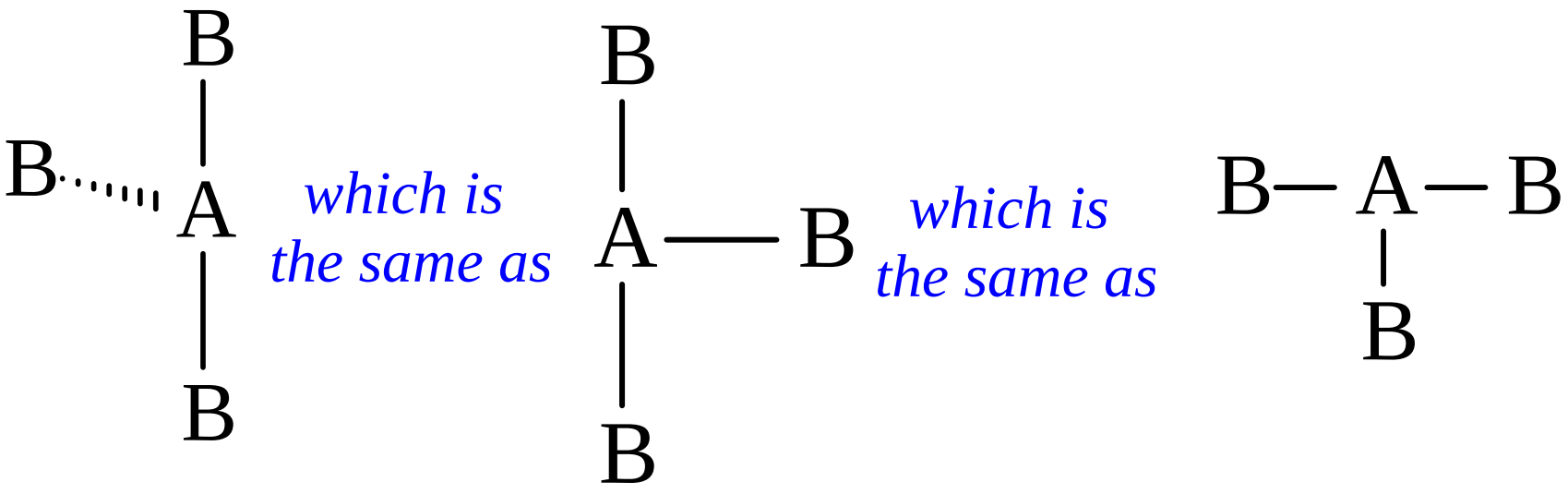
LP-BP Must Determine Best Shape





“Molecular Shape”

"T-shaped"



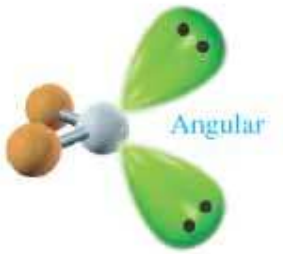
VESPR in Text

TABLE 8-3 *Molecular Geometry of Species with Lone Pairs (U) on the Central Atom*

General Formula	Regions of High Electron Density	Electronic Geometry	Hybridization at Central Atom	Lone Pairs	Molecular Geometry	Examples
AB_2U	3	trigonal planar	sp^2	1		O_3, NO_2^-, SO_2

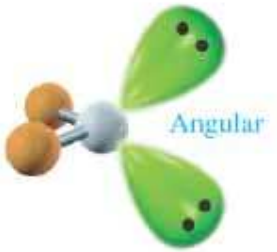
VSEPR cont.

TABLE 8-3 *Molecular Geometry of Species with Lone Pairs (U) on the Central Atom*

General Formula	Regions of High Electron Density	Electronic Geometry	Hybridization at Central Atom	Lone Pairs	Molecular Geometry	Examples
AB_3U	4	tetrahedral	sp^3	1		NH_3, SO_3^{2-}
AB_2U_2	4	tetrahedral	sp^3	2		H_2O, NH_2^-

VSEPR cont.

TABLE 8-3 *Molecular Geometry of Species with Lone Pairs (U) on the Central Atom*

General Formula	Regions of High Electron Density	Electronic Geometry	Hybridization at Central Atom	Lone Pairs	Molecular Geometry	Examples
AB_3U	4	tetrahedral	sp^3	1		NH_3, SO_3^{2-}
AB_2U_2	4	tetrahedral	sp^3	2		H_2O, NH_2^-

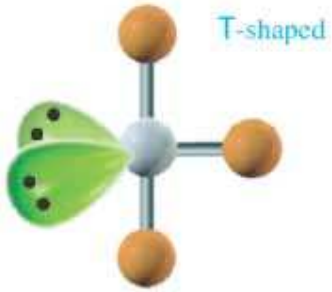
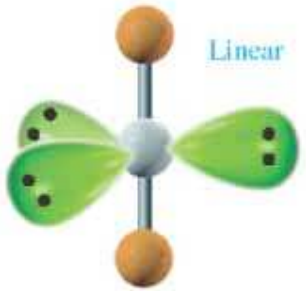
VSEPR cont.

TABLE 8-3 *Molecular Geometry of Species with Lone Pairs (U) on the Central Atom*

General Formula	Regions of High Electron Density	Electronic Geometry	Hybridization at Central Atom	Lone Pairs	Molecular Geometry	Examples
AB_4U	5	trigonal bipyramidal	sp^3d	1		SF_4

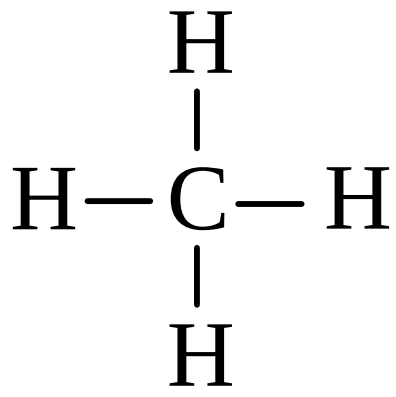
VSEPR cont.

TABLE 8-3 *Molecular Geometry of Species with Lone Pairs (U) on the Central Atom*

General Formula	Regions of High Electron Density	Electronic Geometry	Hybridization at Central Atom	Lone Pairs	Molecular Geometry	Examples
AB_3U_2	5	trigonal bipyramidal	sp^3d	2		ICl_3, ClF_3
AB_2U_3	5	trigonal bipyramidal	sp^3d	3		XeF_2, I_3^-

Hybridization Theory

CH_4

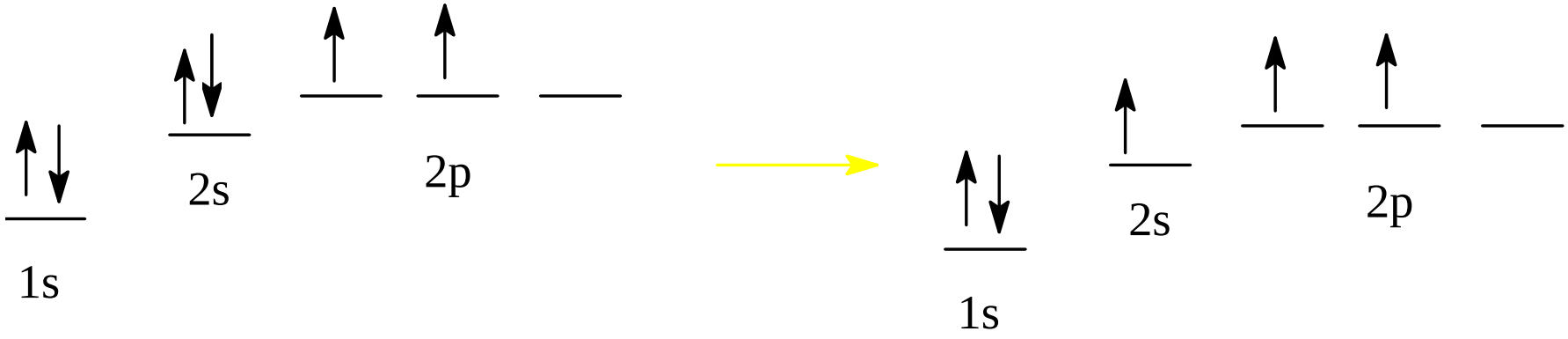


Note: 4 covalent bonds
therefore 4 unpaired electrons
required

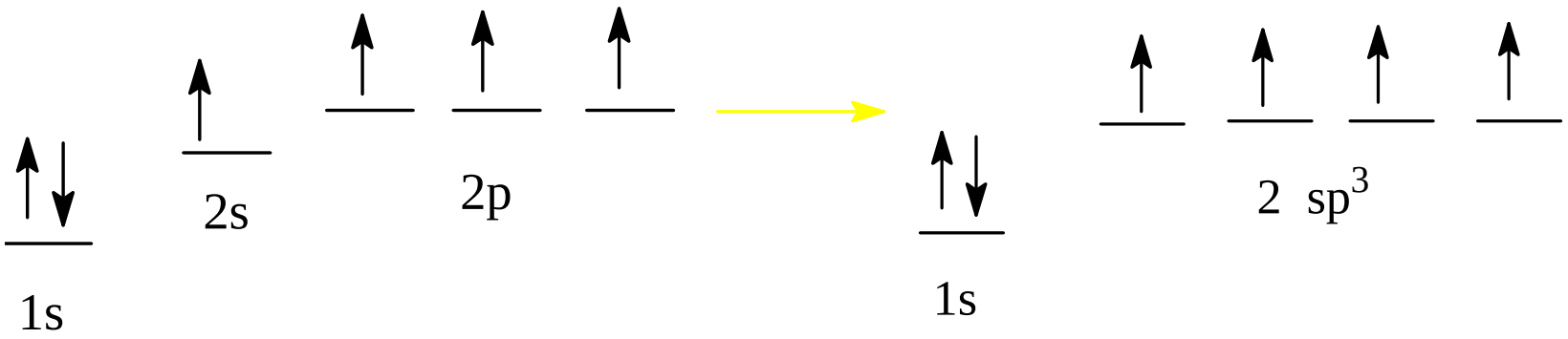
Q1
Ground state electron configuration

$1s^2 2s^2 2p^2$

Step 1- Electron Promotion

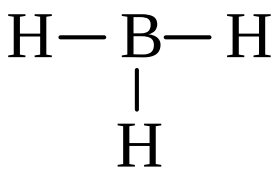


Step 2- Orbital hybridization



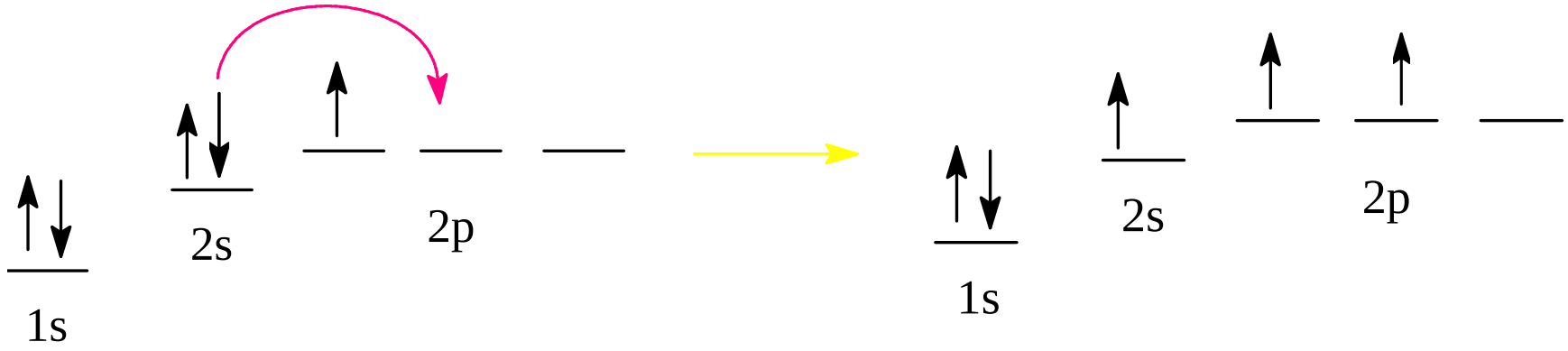
Q2
Boron and hybridization

BH_3

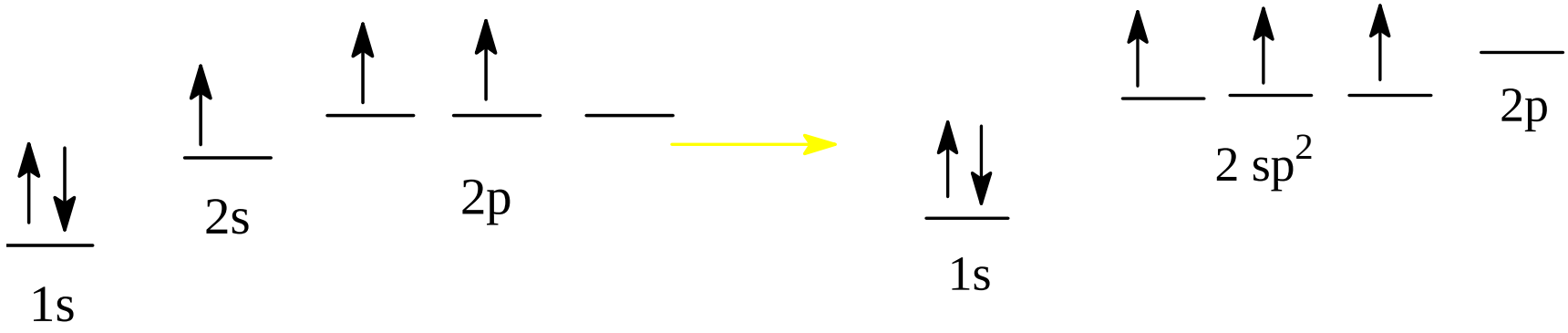


$1s^2 2s^2 2p^1$

First step- electron promotion



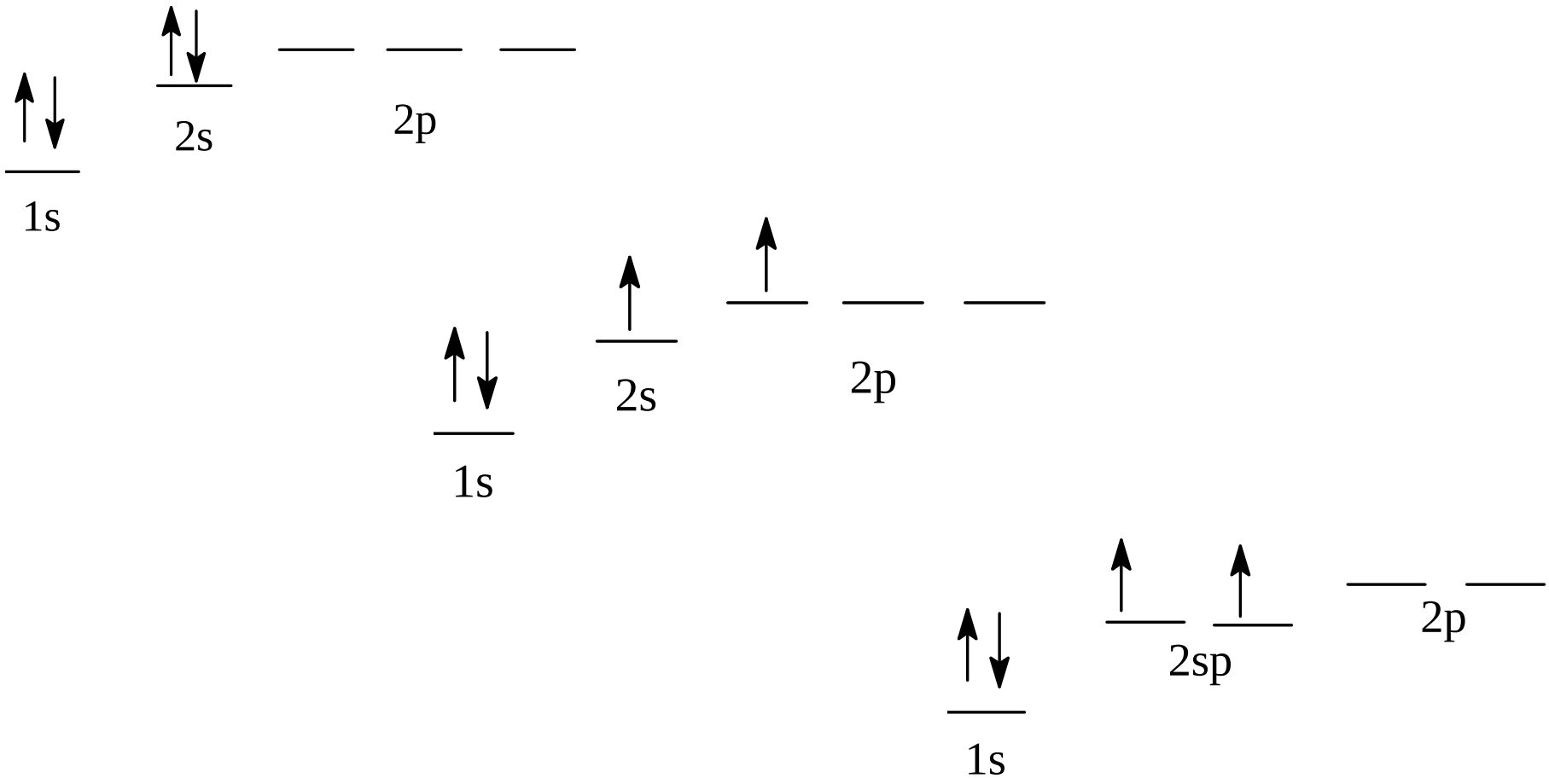
Orbital hybridization



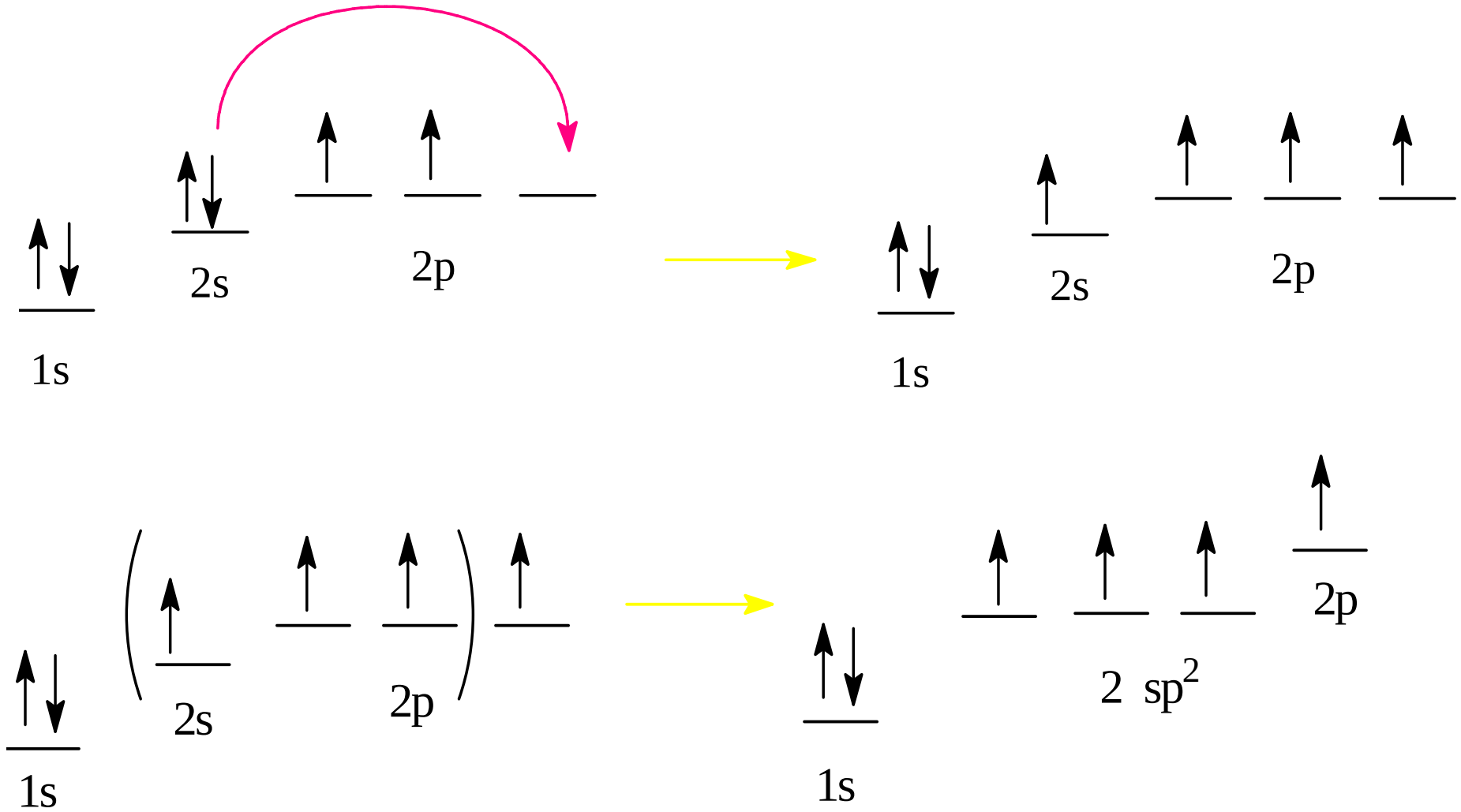
Q3

BeH_2

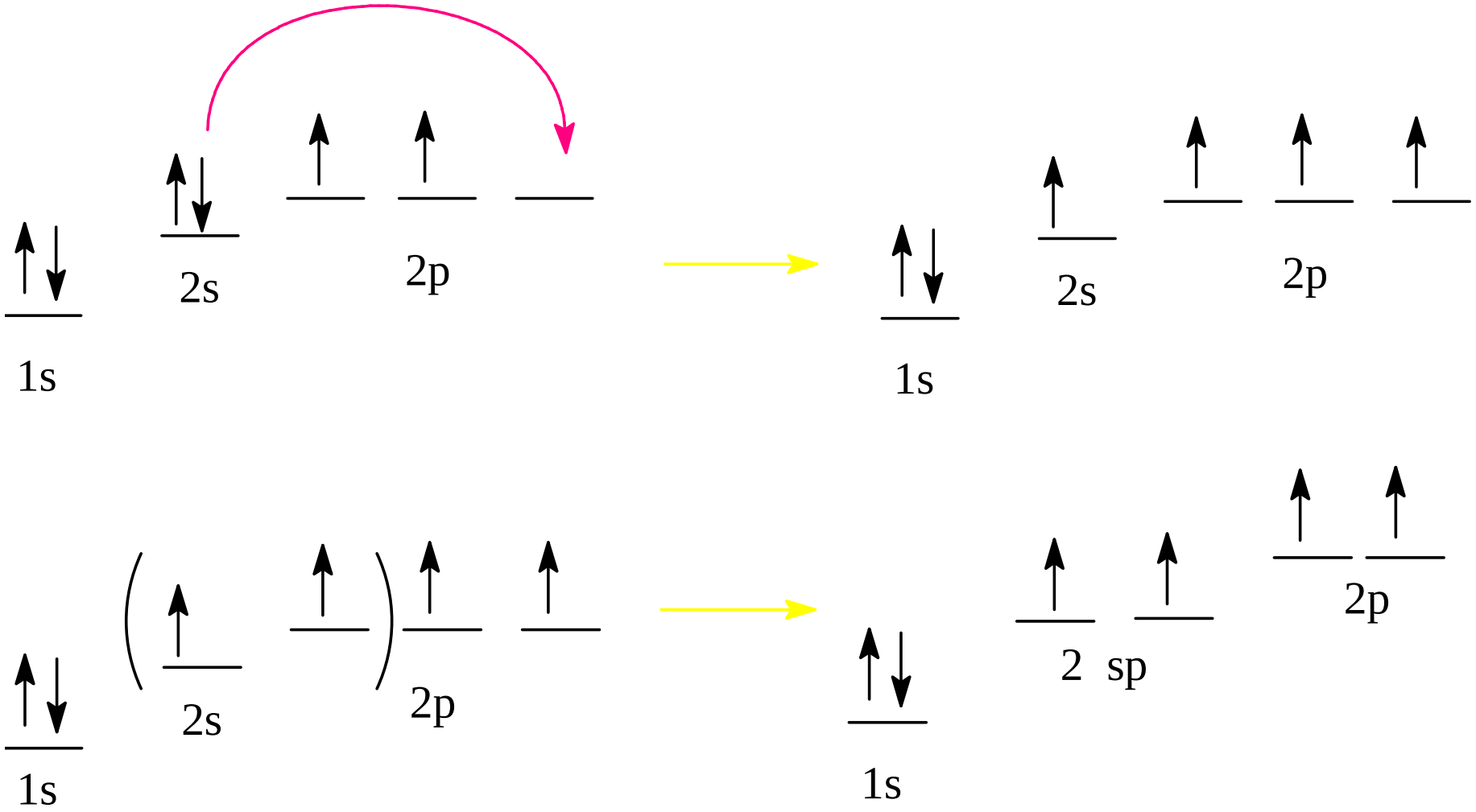
ground state



Sp^2 hybridization of carbon

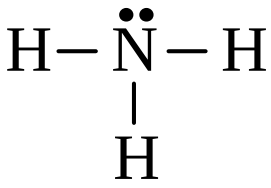


sp hybridization of carbon



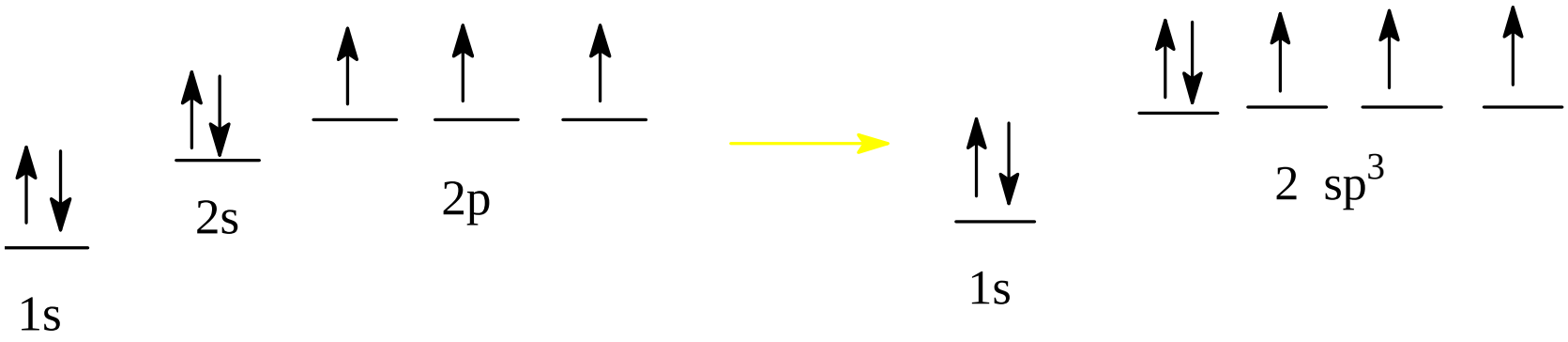
Nitrogen compounds

NH_3



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

Orbital hybridization
(reduces lone pair repulsions)



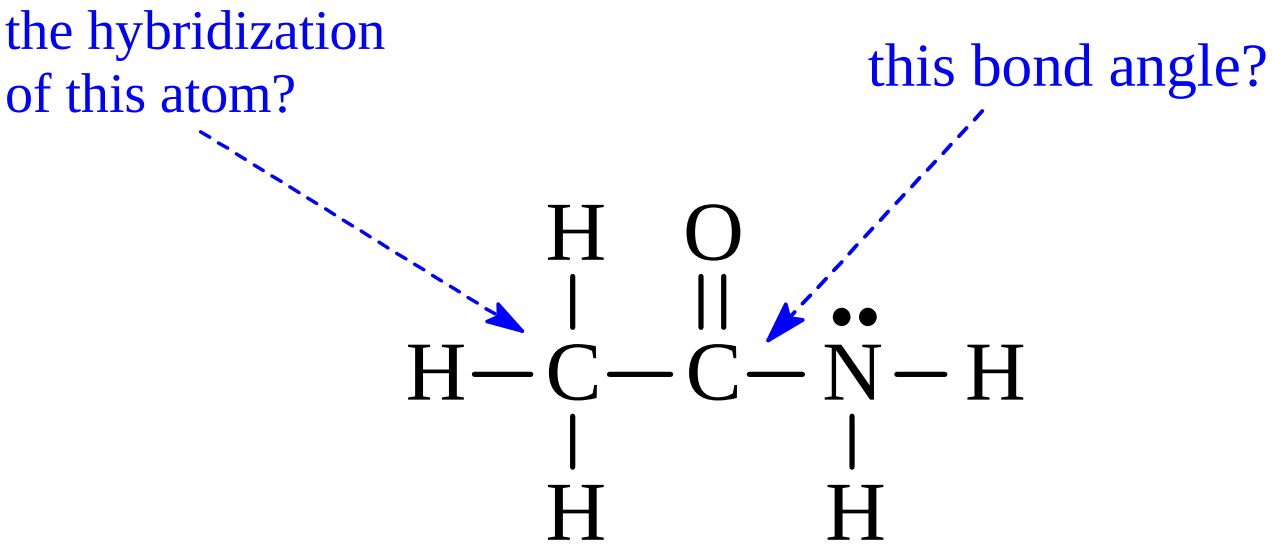
Q4

Try H_2O

VSEPR and Hybridization

count	hybridization	shape
4	**sp^3**	**tetrahedral**
3	**sp^2**	**trigonal planar**
2	**sp**	**linear**

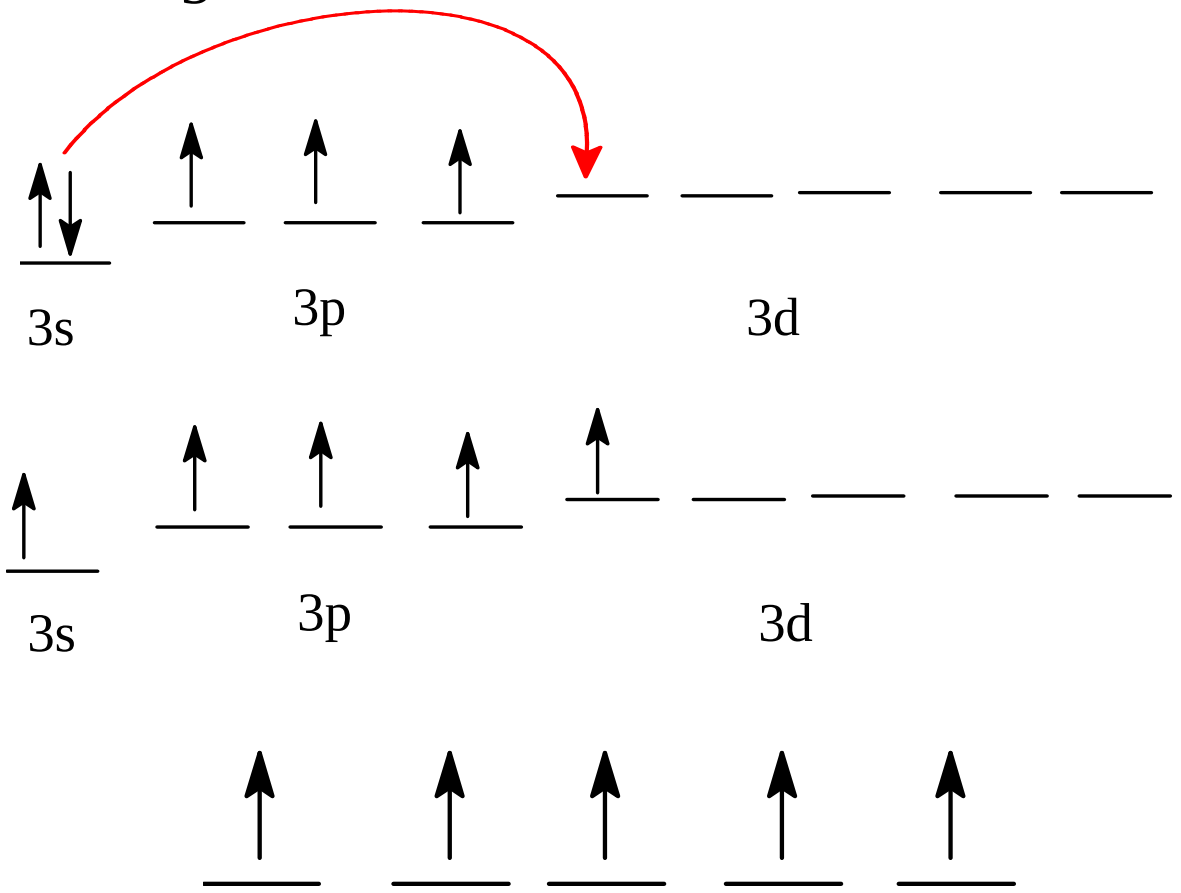
Application



Expanded Octets and Hybridization

PCl_5 as an example

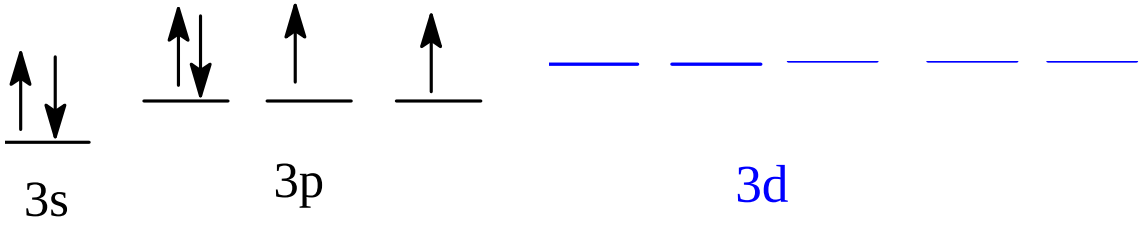
PCl_5



3 **dsp^3**

Q5

SF_6 **$3s^2 3p^4$**

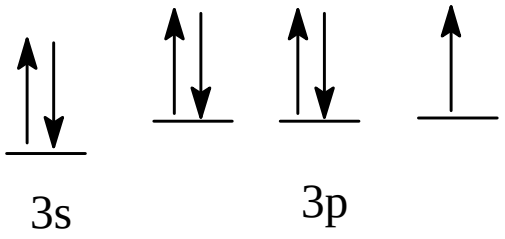


Summary

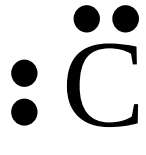
count	hybridization	shape
6	d^2sp^3	octahedral
5	dsp^3	trig. bipyramidal
4	sp^3	tetrahedral
3	sp^2	trigonal planar
2	sp	linear

ClF_3

Cl $3s^2 3p^5$



Results



"AB_3U_2"

Q6

XeF_4

Molecular Shape

Ions

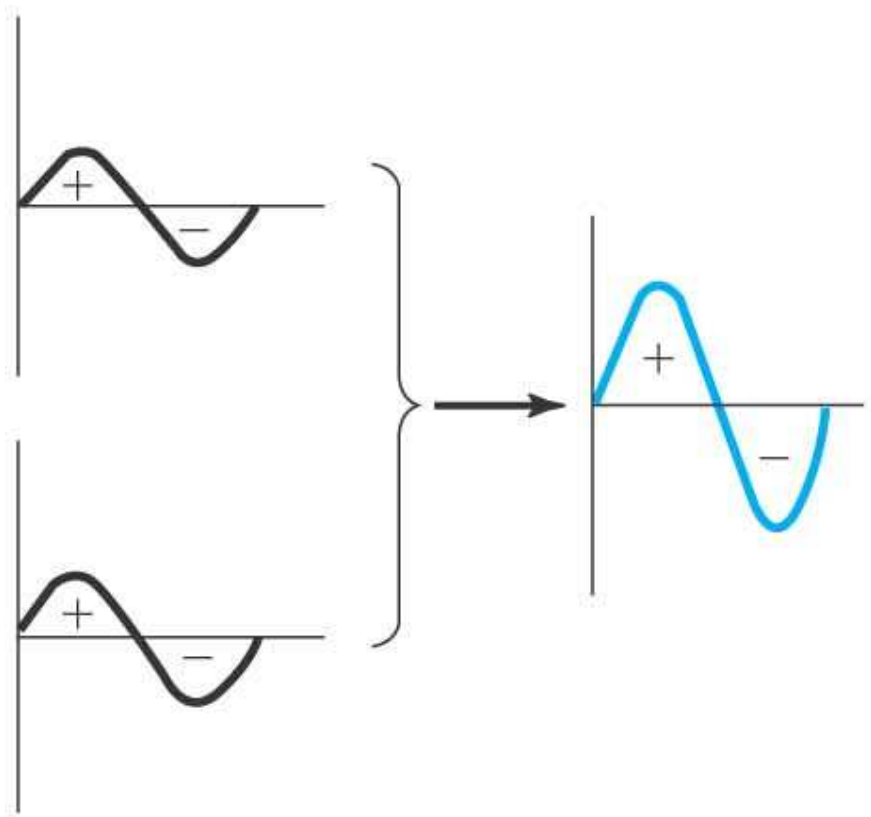
add or remove electrons to central atom **before** hybridizing

$$IF_4^{-1}$$

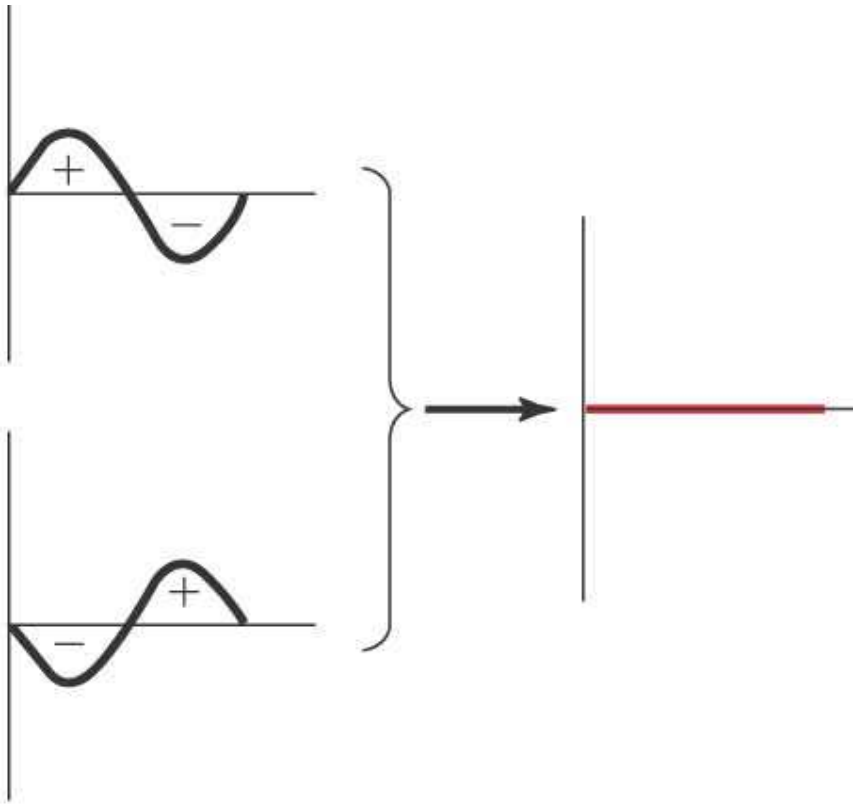
try these

XeF_2 **KrF_3^{+1}** **BrF_5**

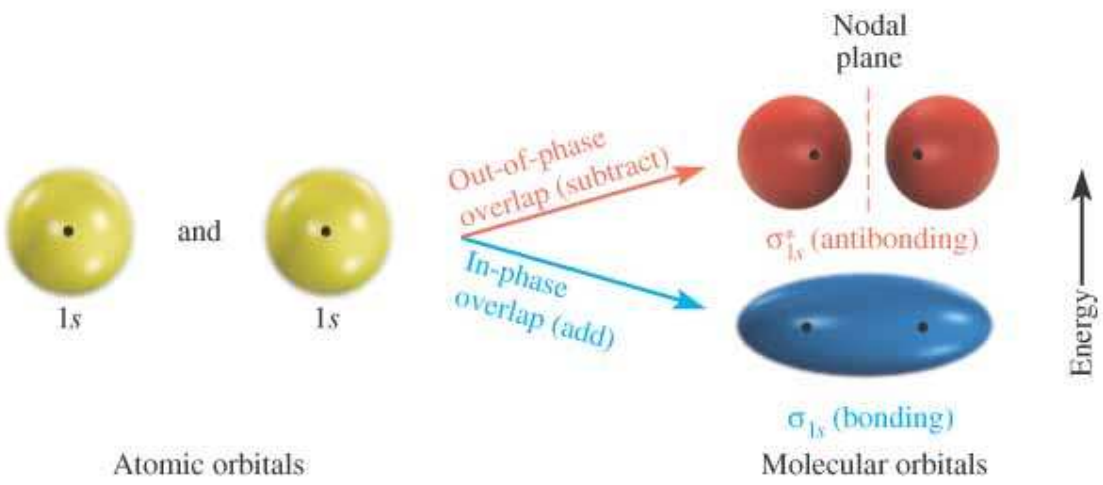
MOs

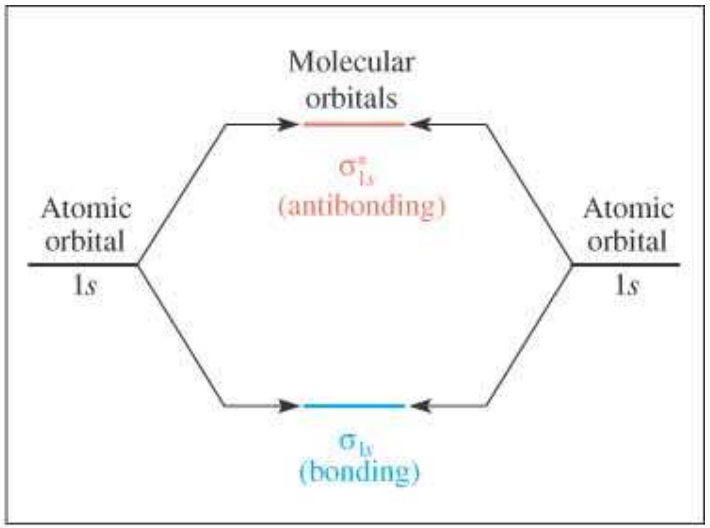


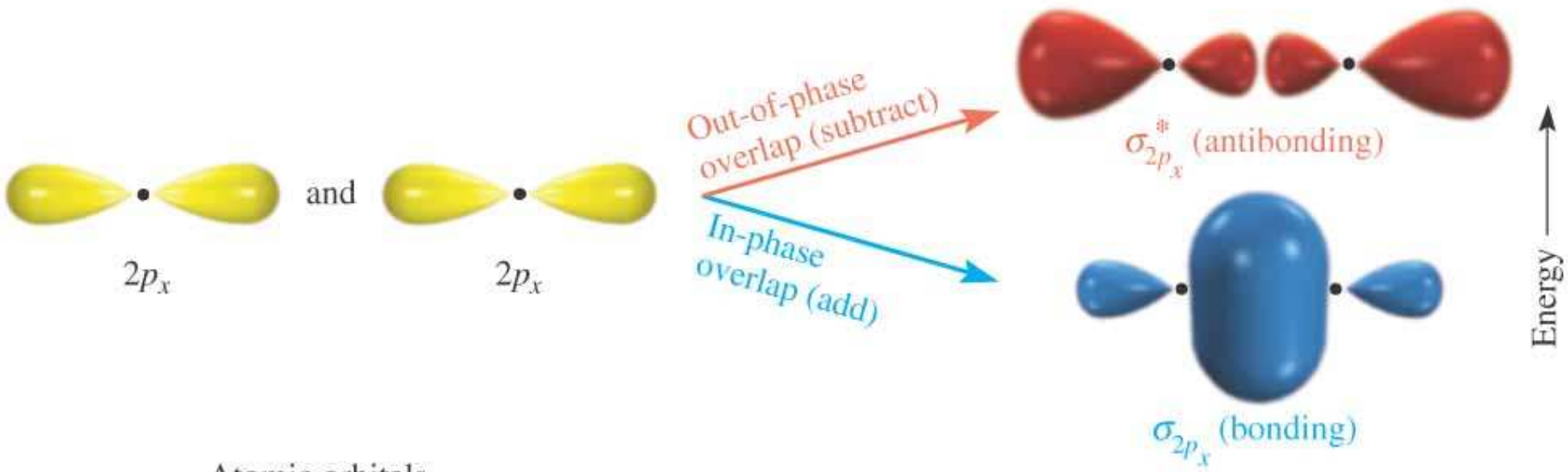
(a) In-phase overlap (add)

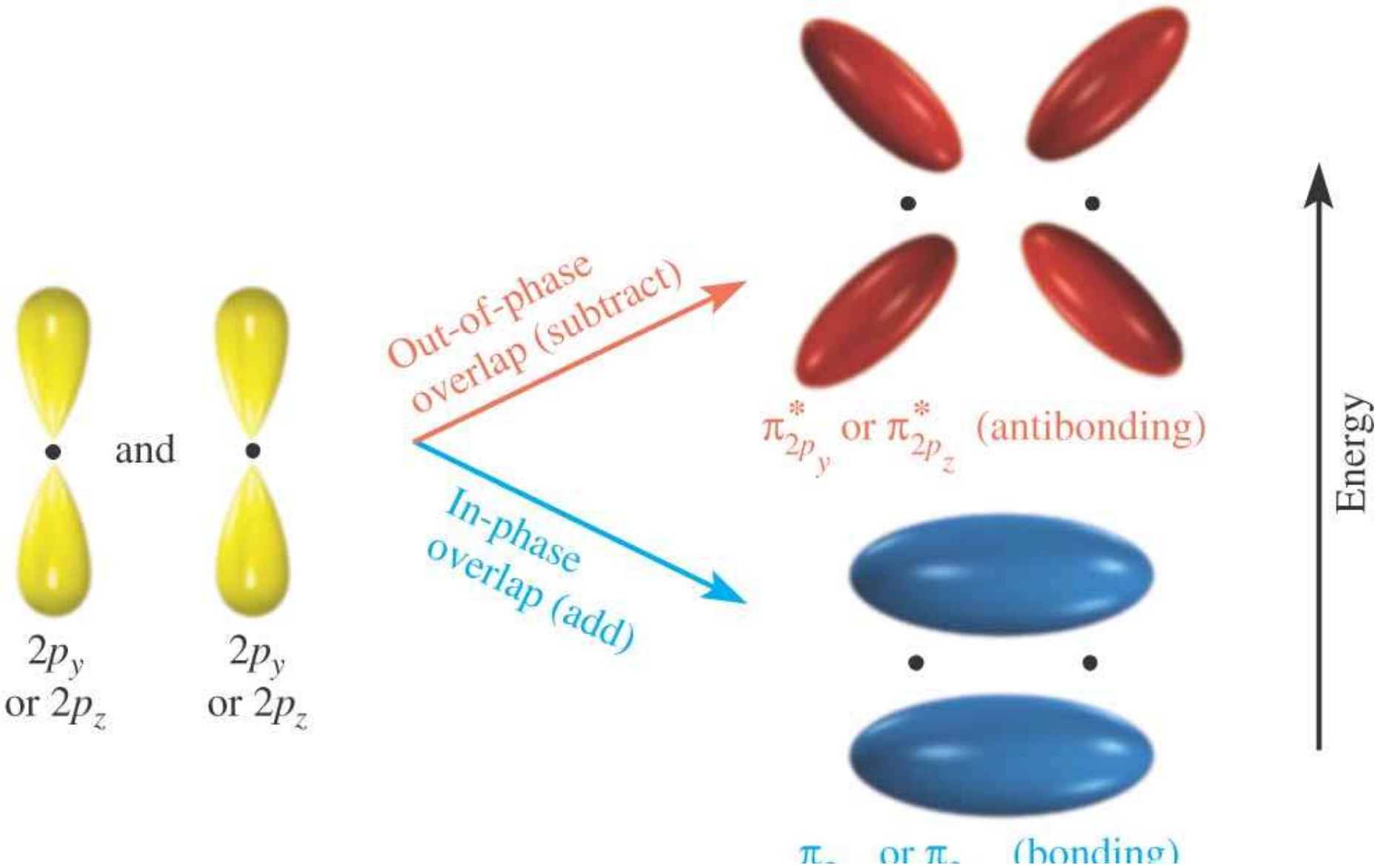


(b) Out-of-phase overlap (subtract)



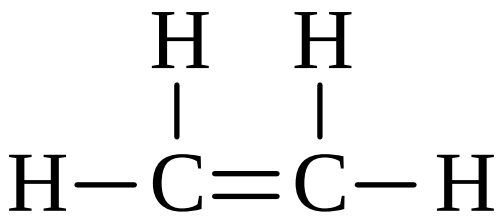




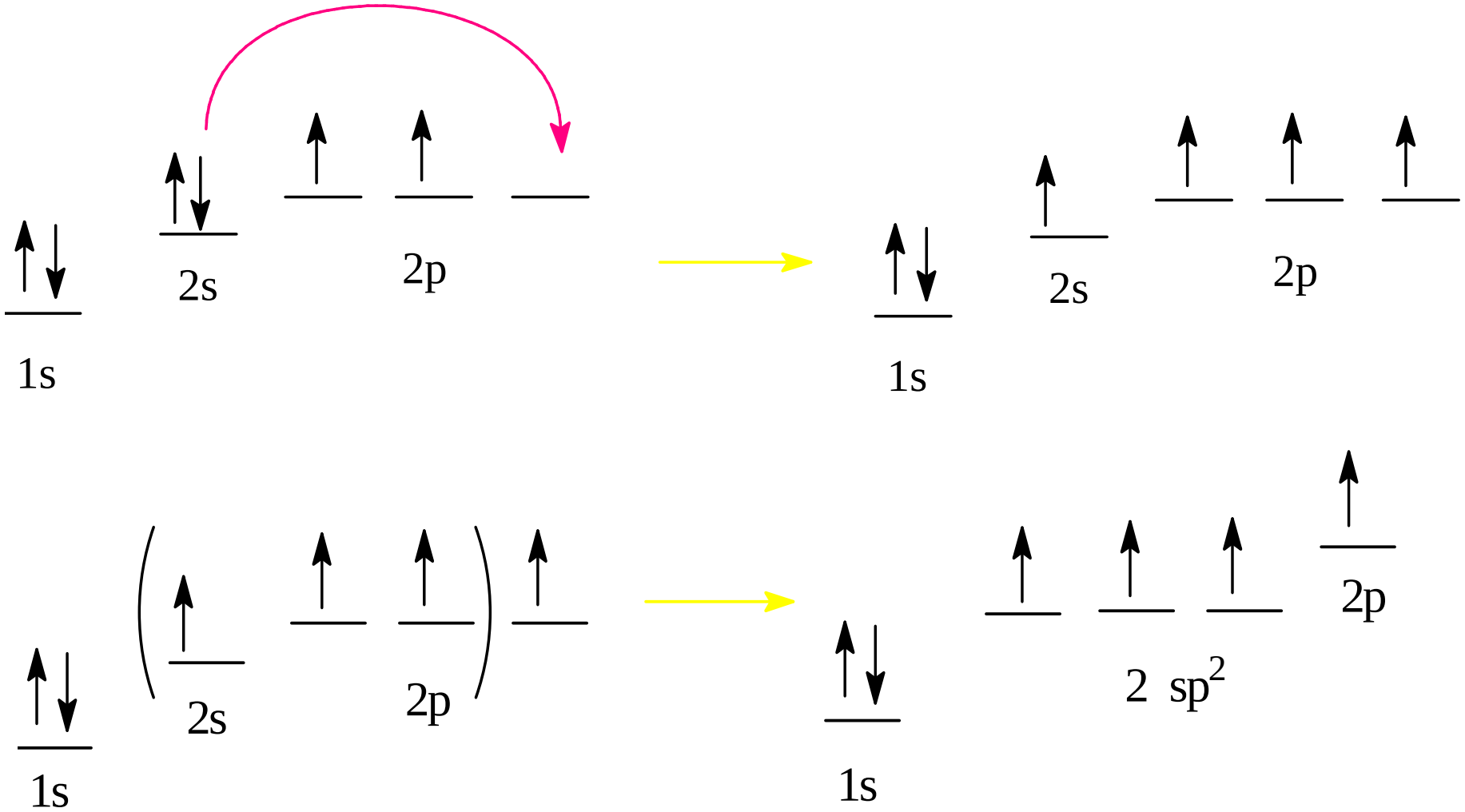

and
$2p_y$ or $2p_z$
$2p_y$ or $2p_z$
Out-of-phase overlap (subtract)
In-phase overlap (add)
$\pi^*_{2p_y}$ or $\pi^*_{2p_z}$ (antibonding)
(bonding)
Energy

Putting it All Together

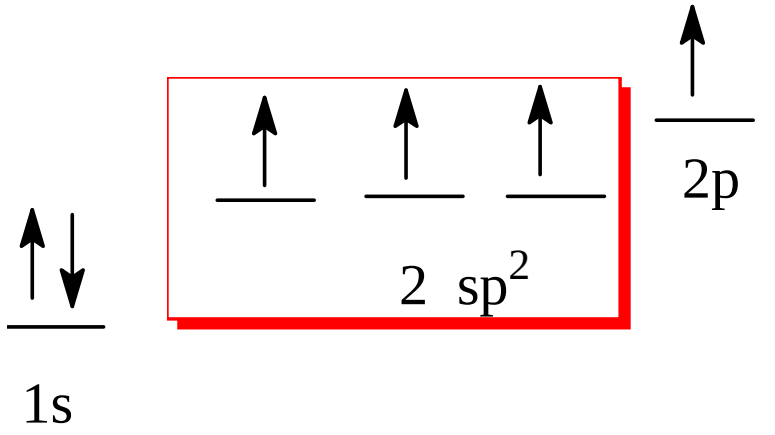
C_2H_4

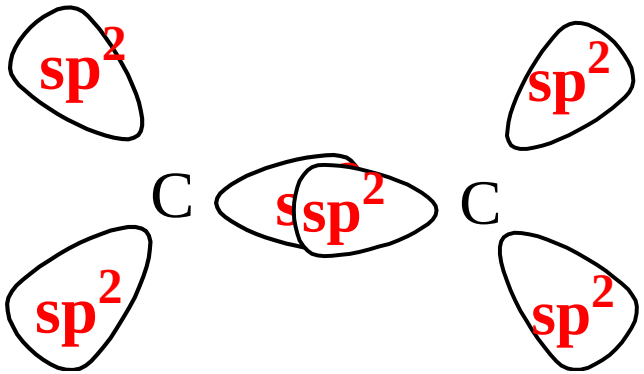


Sp^2 hybridization of carbon

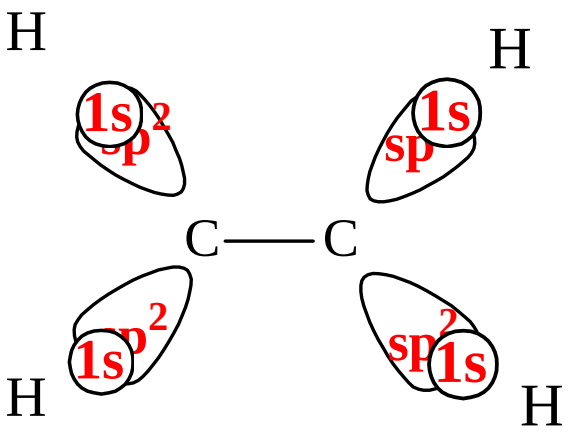


Cont.





Cont.



Cont.