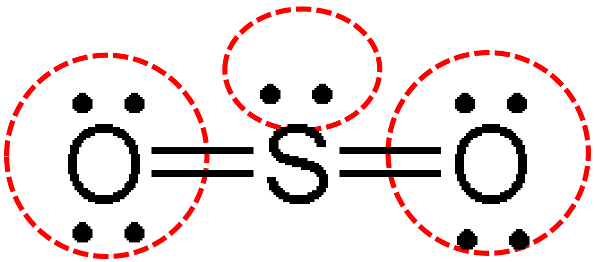
VALENCE BOND THEORY & HYBRIDIZATION

DETERMINING THE HYBRIDIZATION OF ATOMS

Example: $\underline{S}O_2$



1) Count the number of lone pairs and bonded atoms around the atom

3

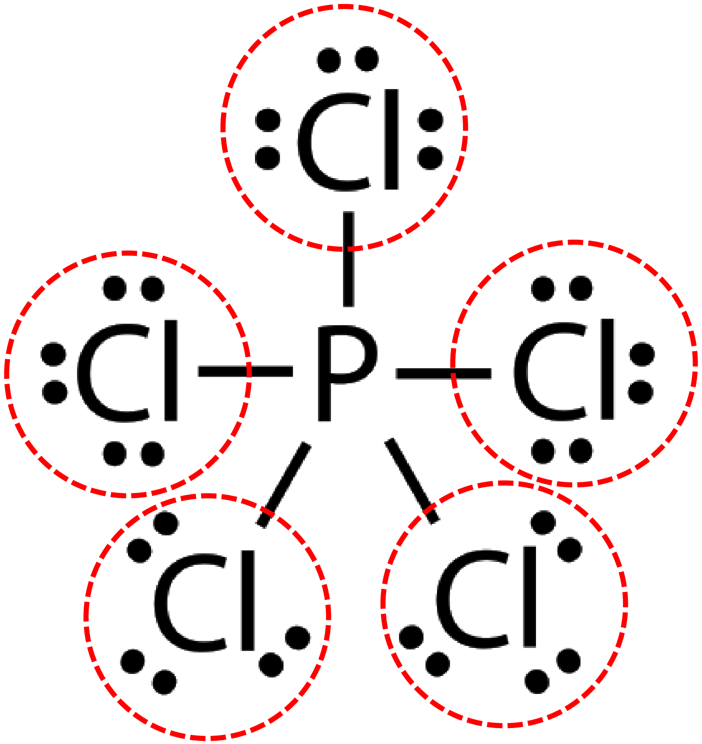
2) Count out the same number with the following sequence in this direction

s p p p d d d d d

.: hybridization of S is sp^2

DETERMINING THE HYBRIDIZATION OF ATOMS

Example: PCl_5



1) Count the number of lone pairs and bonded atoms around the atom

5

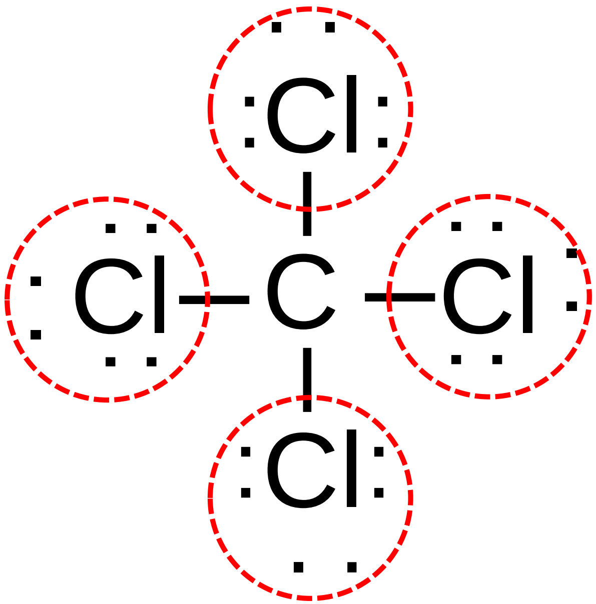
2) Count out the same number with the following sequence in this direction

s p p p d d d d d

.: hybridization of P is sp^3d

DETERMINING THE HYBRIDIZATION OF ATOMS

Example: $\underline{C}Cl_4$



1) Count the number of lone pairs and bonded atoms around the atom

4

2) Count out the same number with the following sequence in this direction

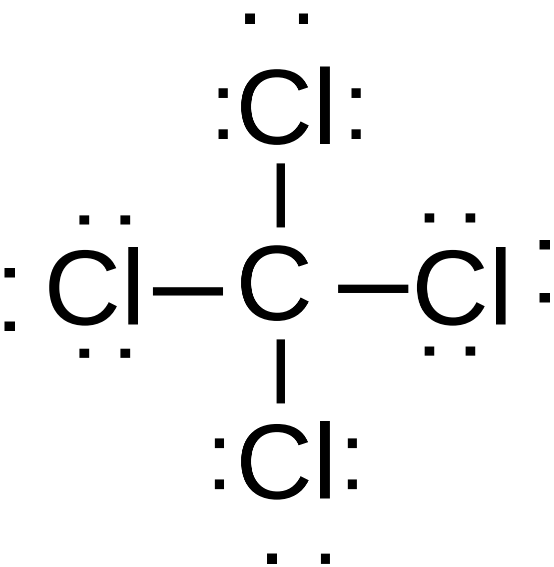
s p p p d d d d d

.: hybridization of C is sp^3

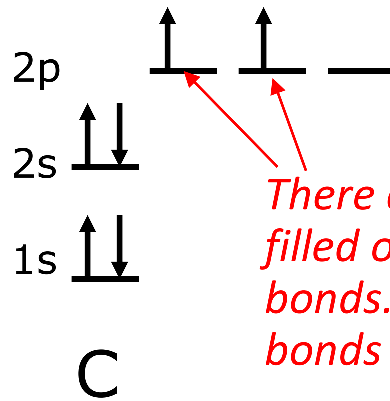
EXPLAINING BONDING WITH HYBRIDIZATION

Example: CCl_4

How does **sp³** hybridization explain how carbon bonds in CCl_4?



Energy level diagram of carbon:



There are only 2 half-filled orbitals to form bonds. How do we get 4 bonds out of this?

A covalent bond forms when two <u>half-filled</u> orbitals overlap (i.e. ↑↓) to produce a new combined orbital containing two electrons of opposite spin.

EXPLAINING BONDING WITH HYBRIDIZATION

A covalent bond forms when two <u>half-filled</u> orbitals overlap (i.e. $\underline{\uparrow\downarrow}$) to produce a new combined orbital containing two electrons of opposite spin.

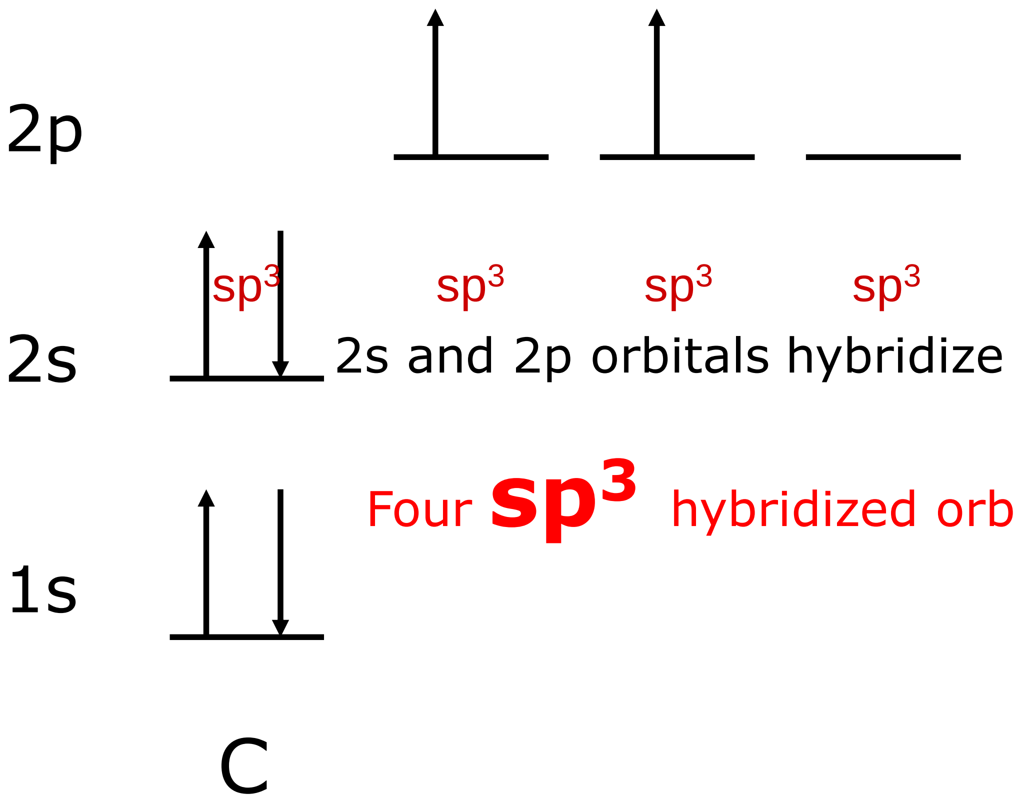
Linus Pauling: **Valence Bond Theory**

- This overlapping results in a decrease in the energy of the atoms forming the bond
- The shared electron pair is most likely to be found in the space between the two nuclei of the atoms forming the bonds.

EXPLAINING BONDING WITH HYBRIDIZATION

Example: $\underline{C}Cl_4$

The orbitals can **hybridize** with each other to form 4 bonds:



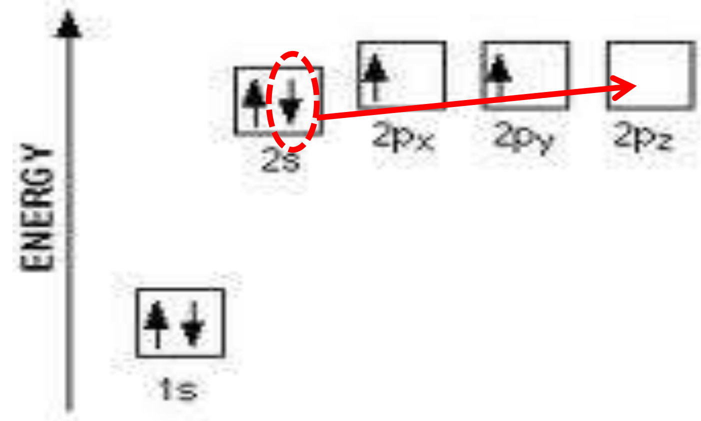
Four **sp^3** hybridized orbitals are formed

HYBRIDIZATION THEORY

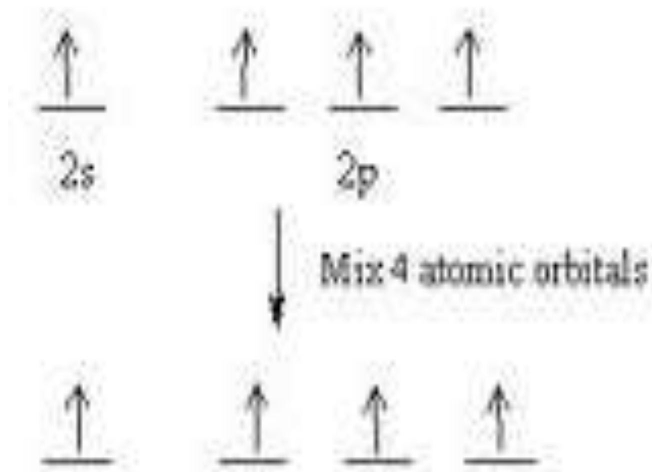
- The Hybridization Theory provides a description of the process involving the combination of atomic orbitals to create new bonding orbitals

- A hybrid orbital is created by combining at least two different orbitals to produce maximum bonding opportunities

- Hybrid orbitals are created through the promotion of electrons



One of carbons 2s electrons is promoted to the empty 2p orbital

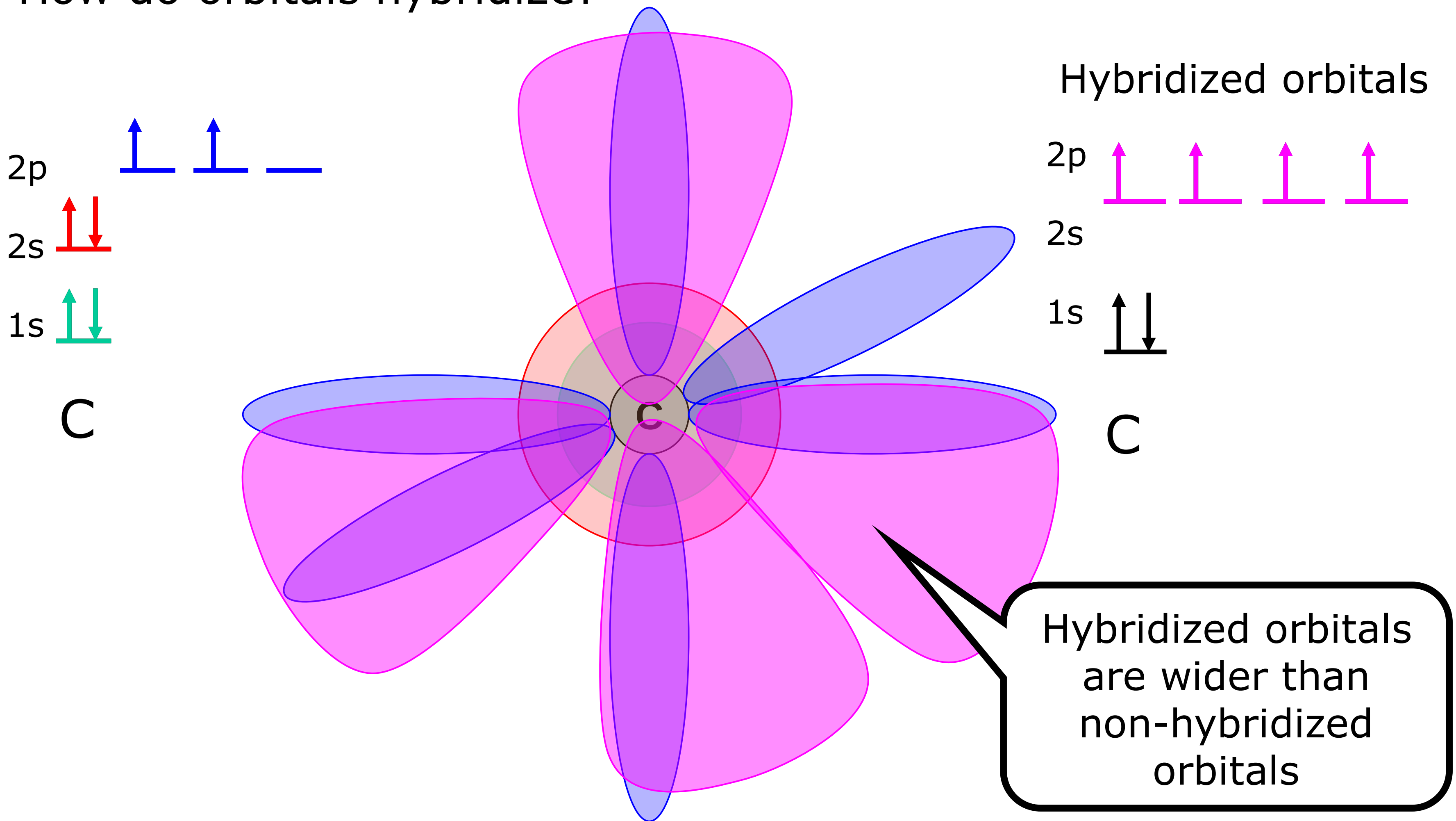


The result produces 4 unpaired electrons for bonding

EXPLAINING HYBRIDIZATION

Example: $\underline{C}Cl_4$

How do orbitals hybridize?



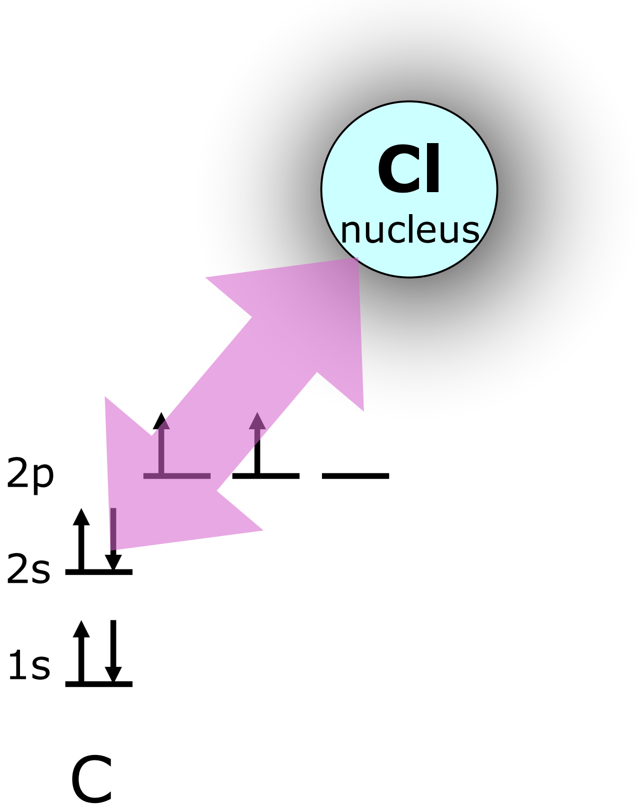
EXPLAINING HYBRIDIZATION

Example: $\underline{C}Cl_4$

What really happens?

The nucleus of a chlorine atom attracts one of the lower-energy valence electrons on carbon.

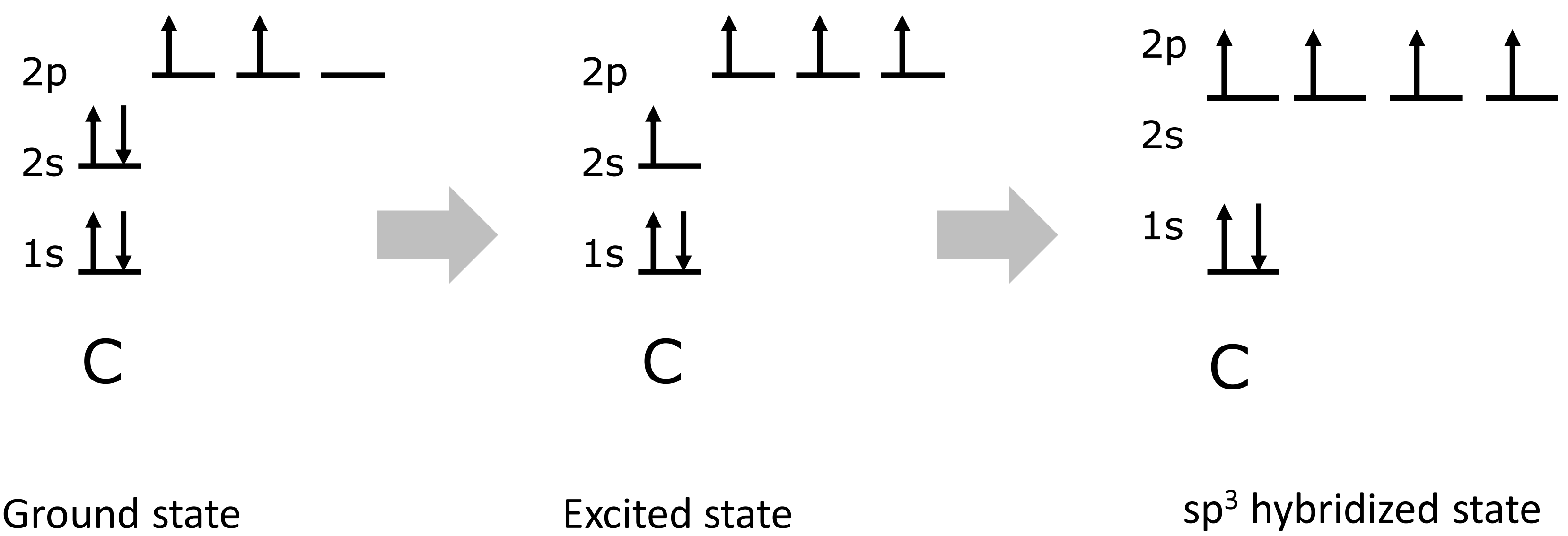
This causes an excitation, moving a 2s electron into a 2p orbital. This, however, increases the attraction of the carbon nucleus on the valence electrons (since the nucleus is slightly less shielded)



EXPLAINING HYBRIDIZATION

Example: $\underline{C}Cl_4$

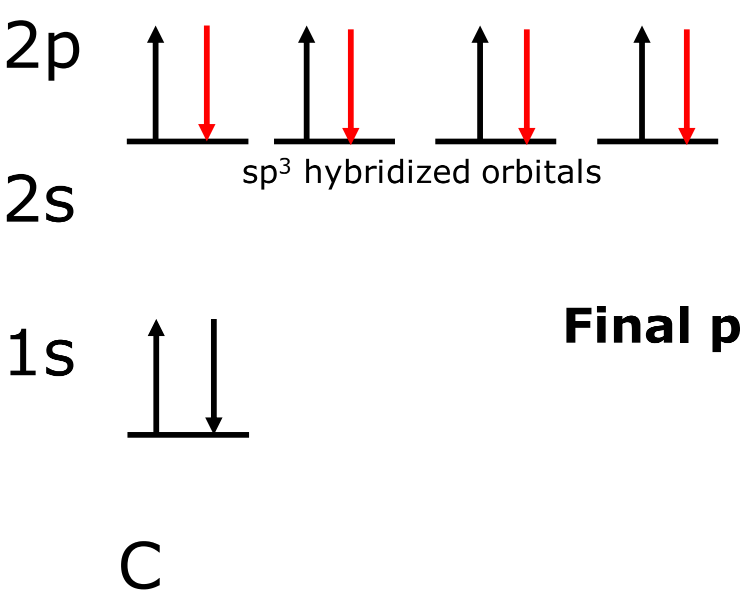
What really happens?



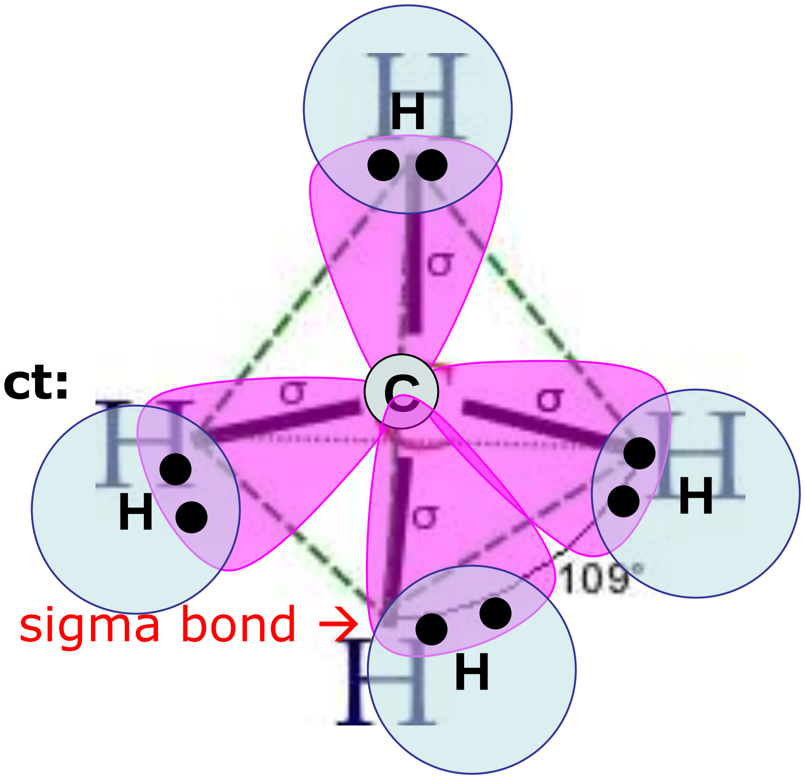
EXAMPLE: METHANE

Example: CH_4

4 hydrogen atoms bond, thus filling every orbital to make a stable product



Final product:



SIGMA AND PI BONDS

σ-bond

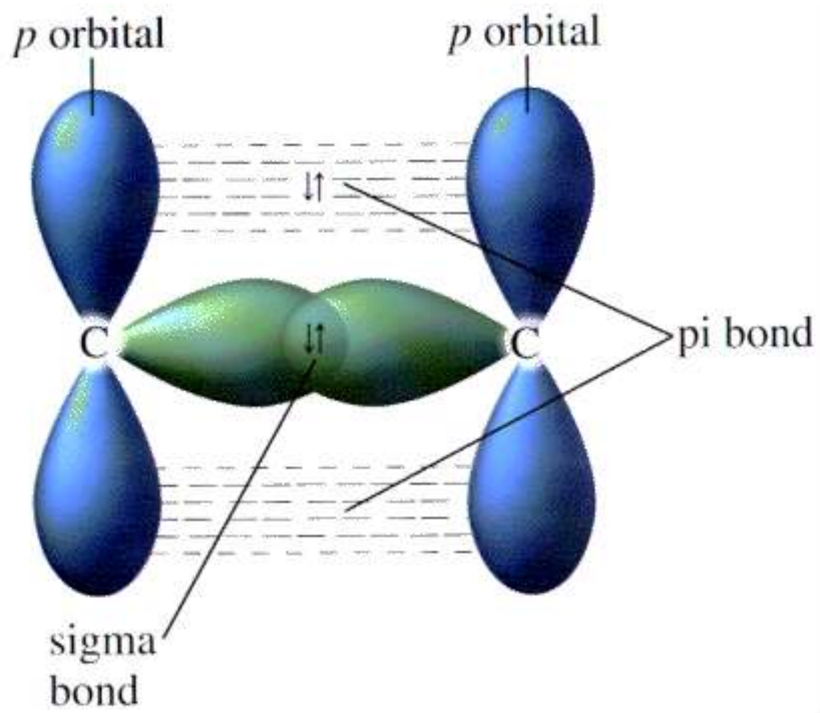
A sigma bond (σ-bond) is a bond formed by the overlap of orbitals in an end-to-end fashion

- electron density is concentrated between the nuclei of the bonding atoms

π-bond

A pi bond (π bond) is a bond formed by the overlap of orbitals in a side-by-side fashion

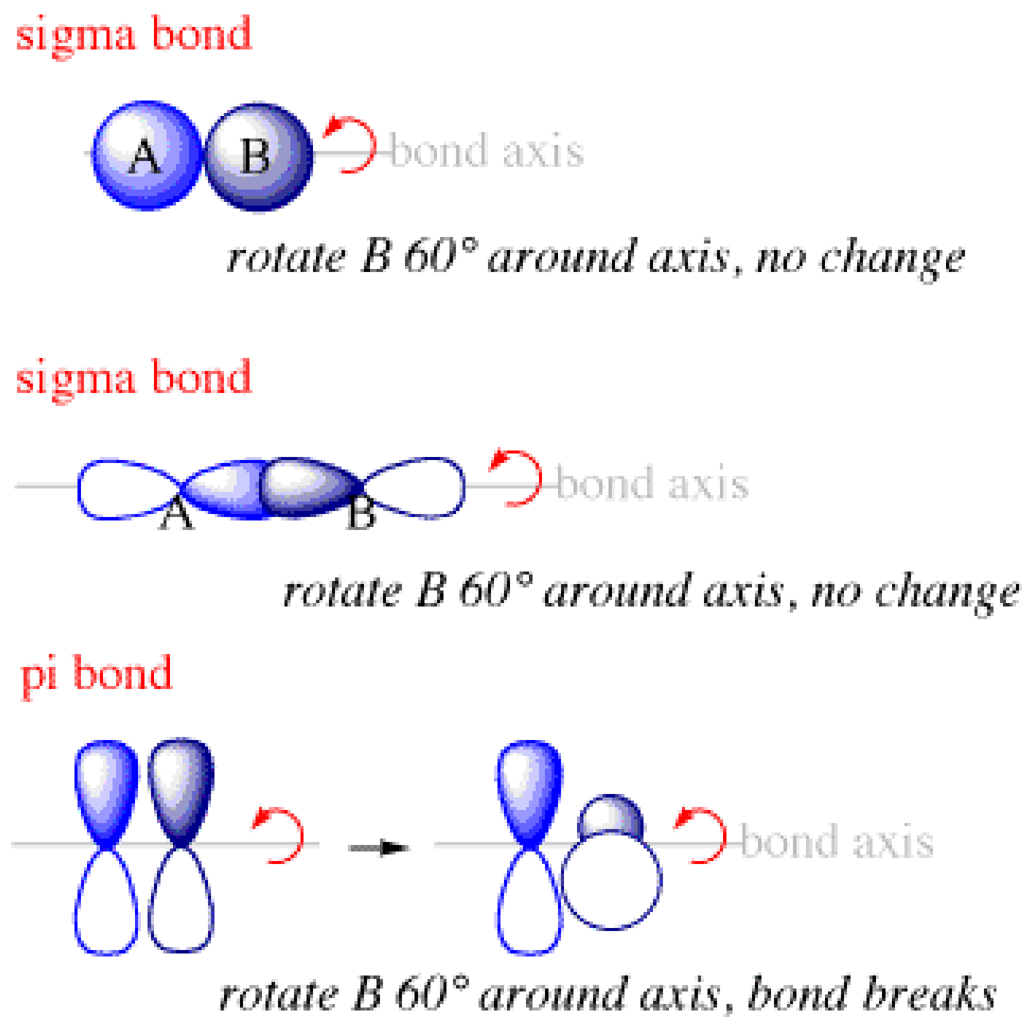
- electron density concentrated above and below the plane of the nuclei of the bonding atoms



SIGMA AND PI BONDS

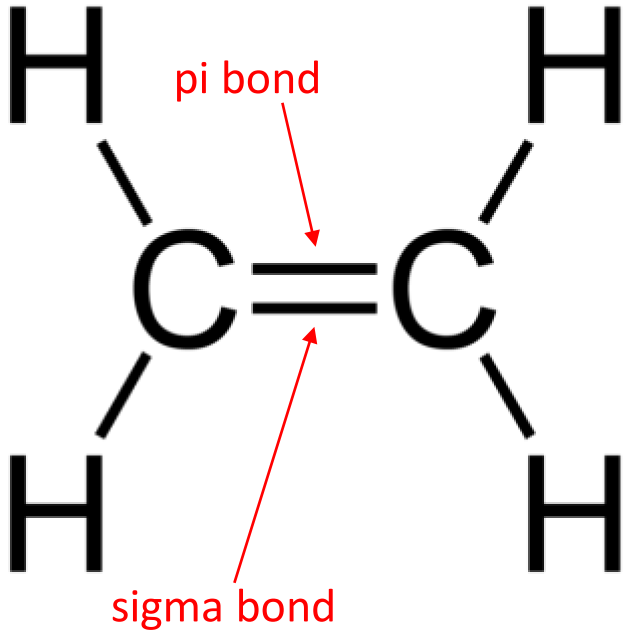
A sigma bond allows free rotation.

A pi bond does not allow free rotation



EXAMPLE: ETHENE

Example: C_2H_4



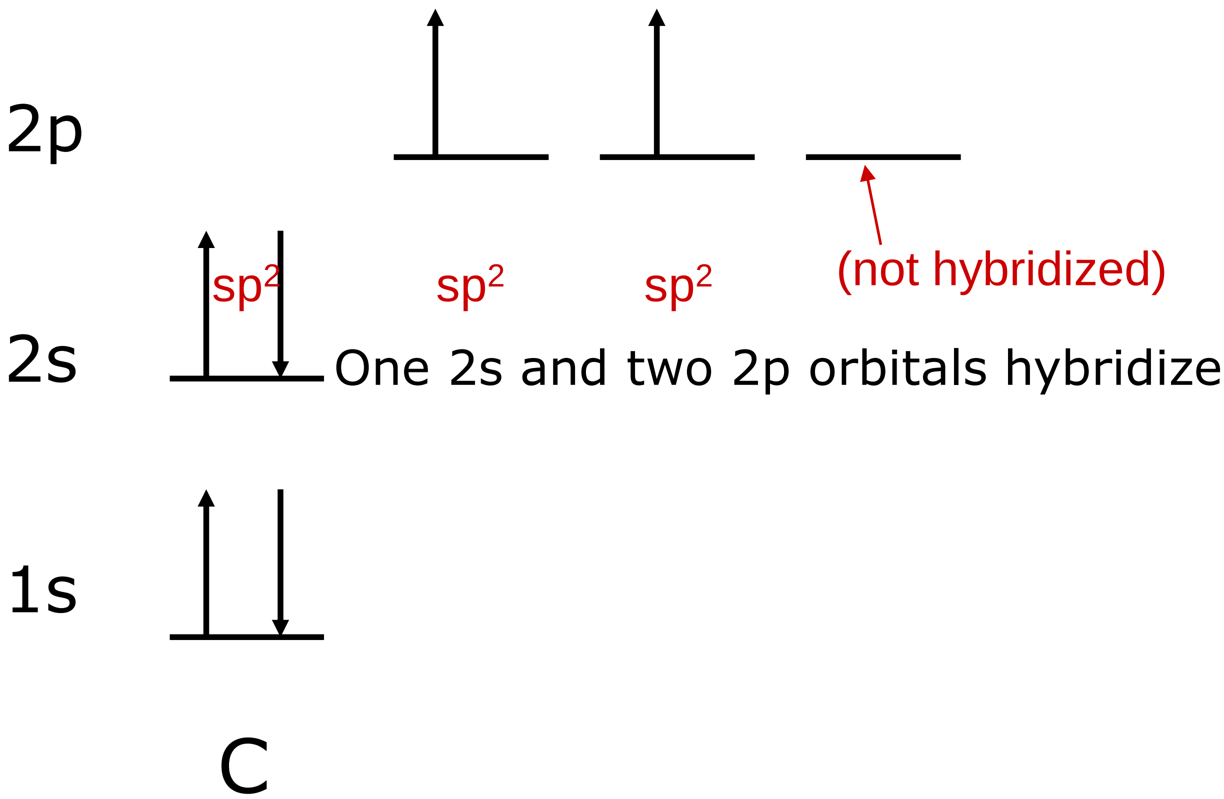
-Double bonds are composed of a sigma bond (end-to-end) and a pi (π) bond (side-by-side overlap)

-pi are covalent bonds, but are weaker than sigma bonds (require less energy to break)

EXAMPLE: ETHENE

Example: C_2H_4

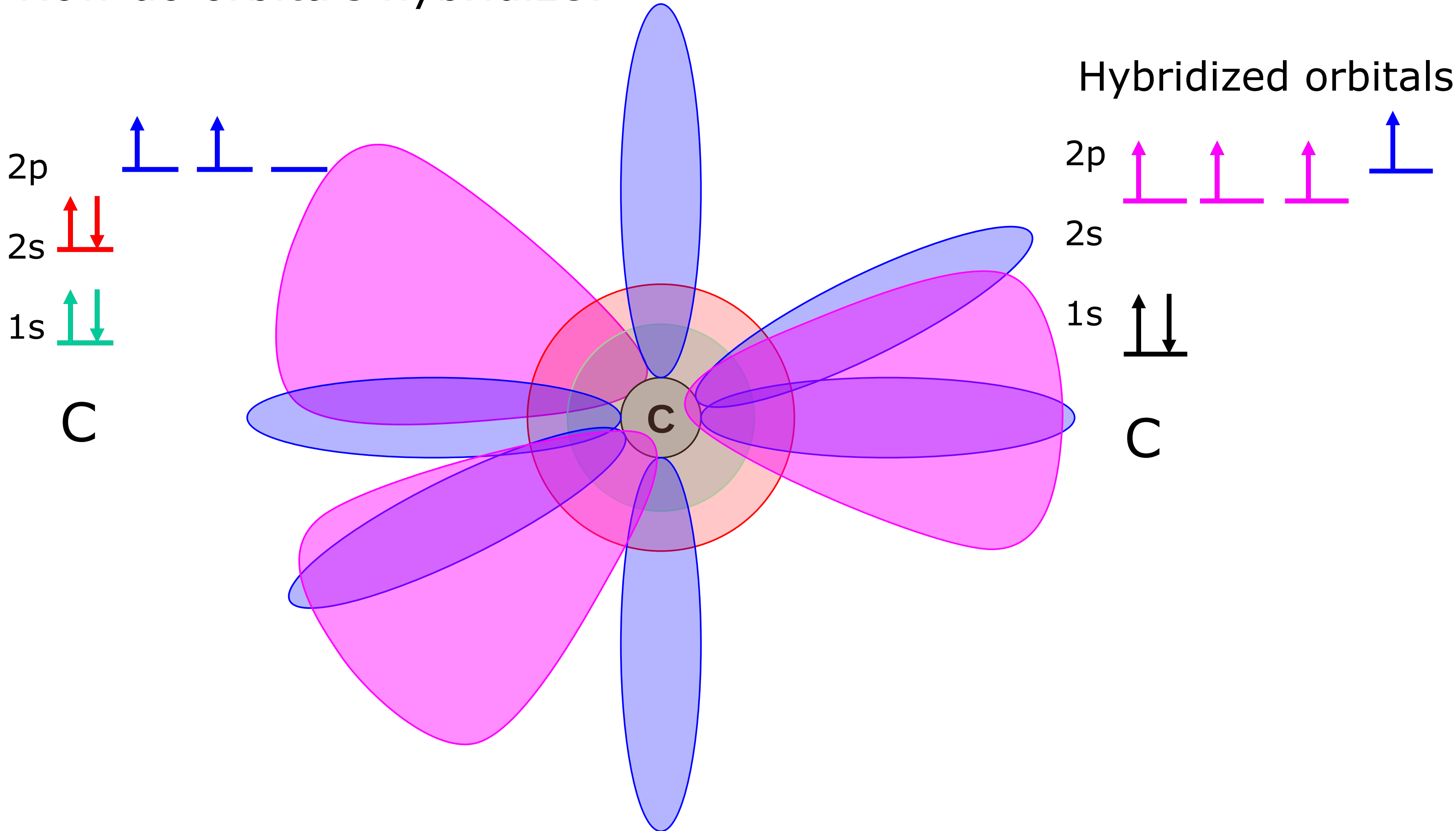
The orbitals will **hybridize** to make 3 sigma bonds + 1 pi bond:



EXAMPLE: ETHENE

Example: **Ethene (C_2H_4)**

How do orbitals hybridize?

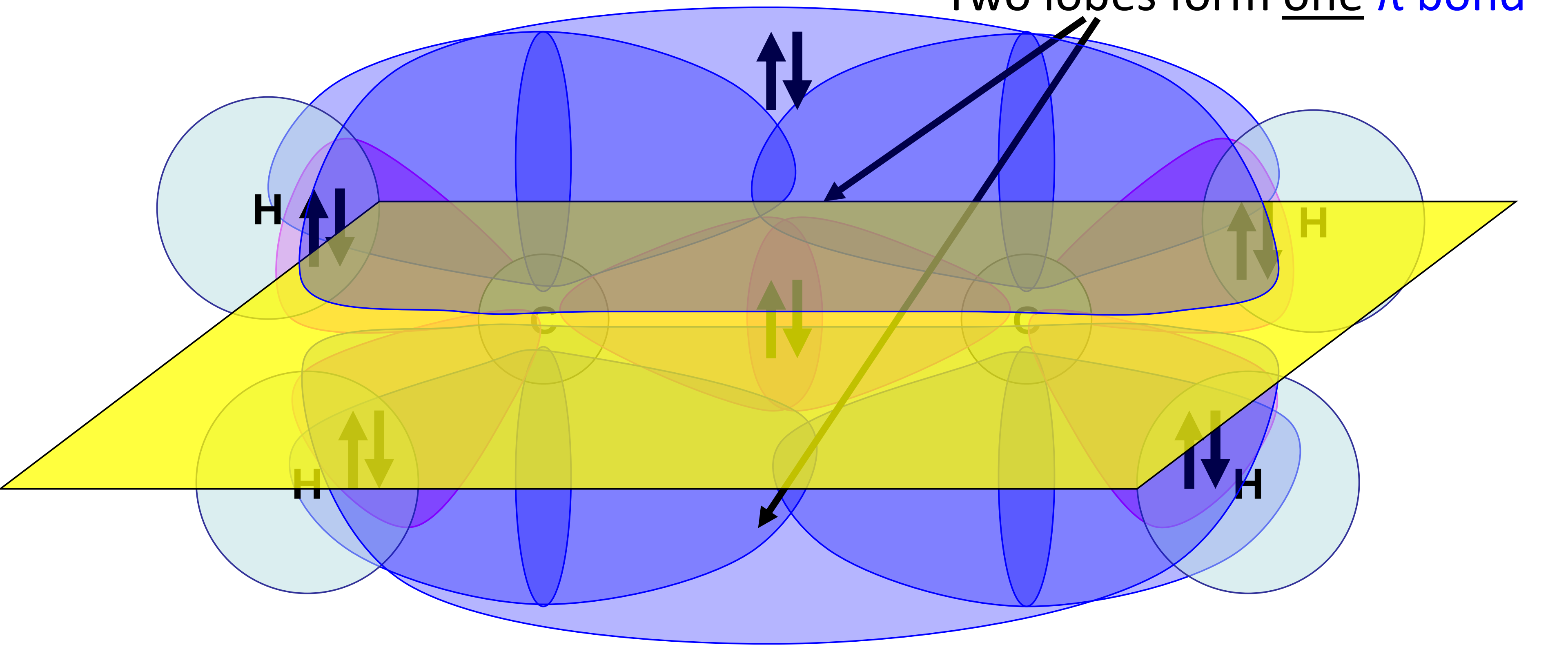


EXAMPLE: ETHENE

Example: C_2H_4

How do the carbons bond in ethene?

Two lobes form <u>one</u> π bond

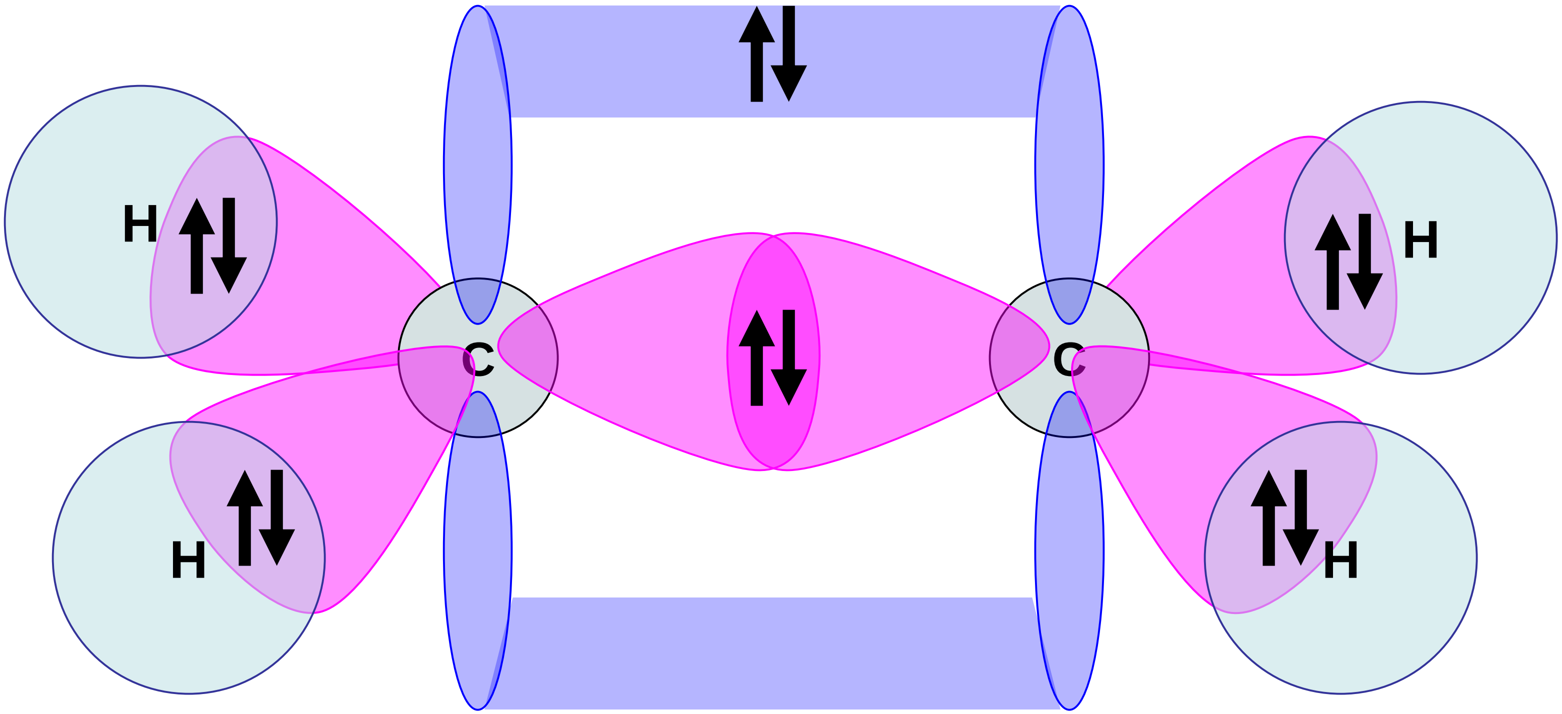


The π bond is symmetrical and above the plane and prevents rotation around the axis between the carbon atoms

EXAMPLE: ETHENE

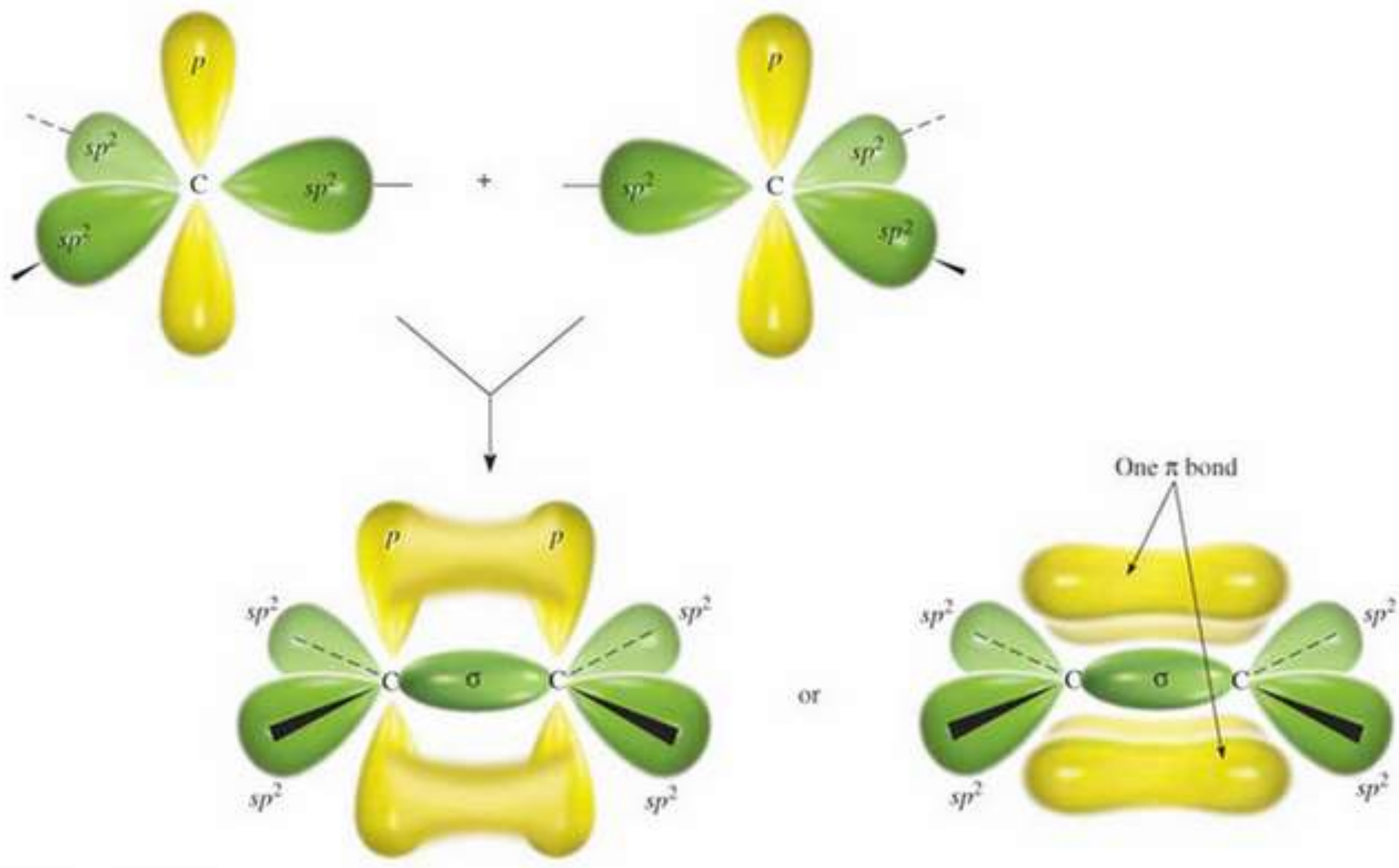
Example: C_2H_4

To draw it more simply…



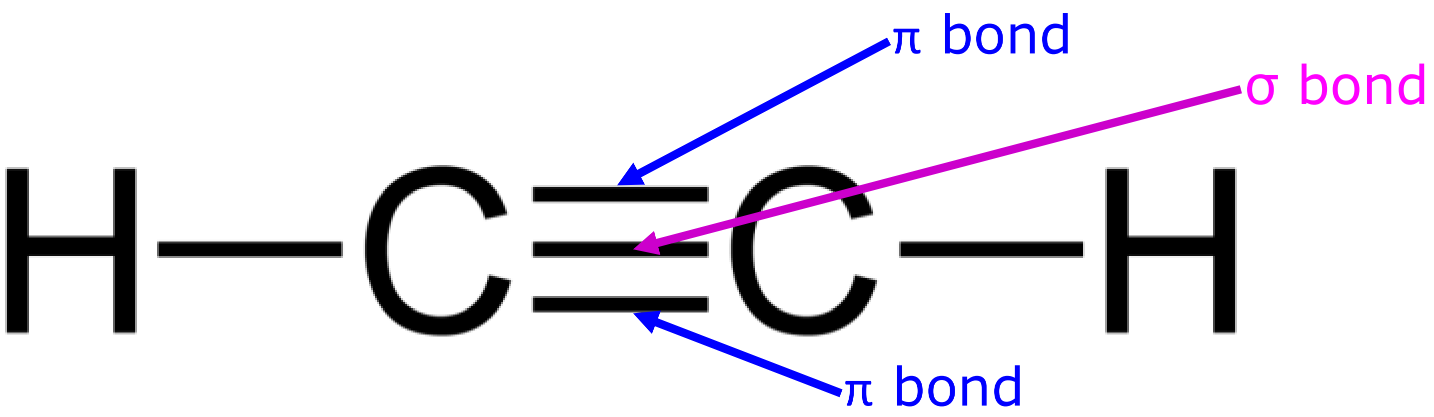
EXAMPLE: ETHENE

Example: C_2H_4



EXAMPLE: ETHYNE

Example: C_2H_2

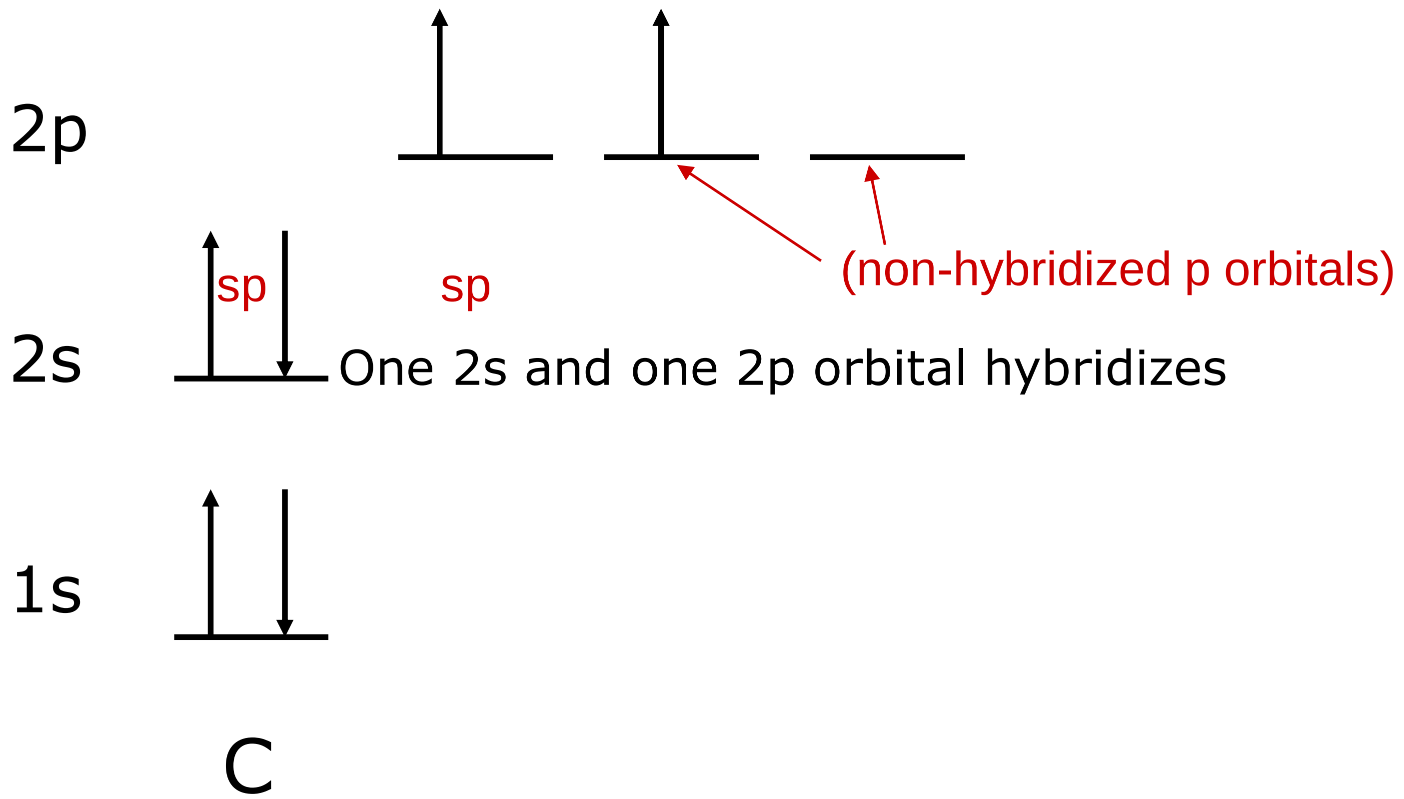


Triple bonds are composed of a sigma bond (end-to-end) and two pi (π) bonds (side-by-side)

EXAMPLE: ETHYNE

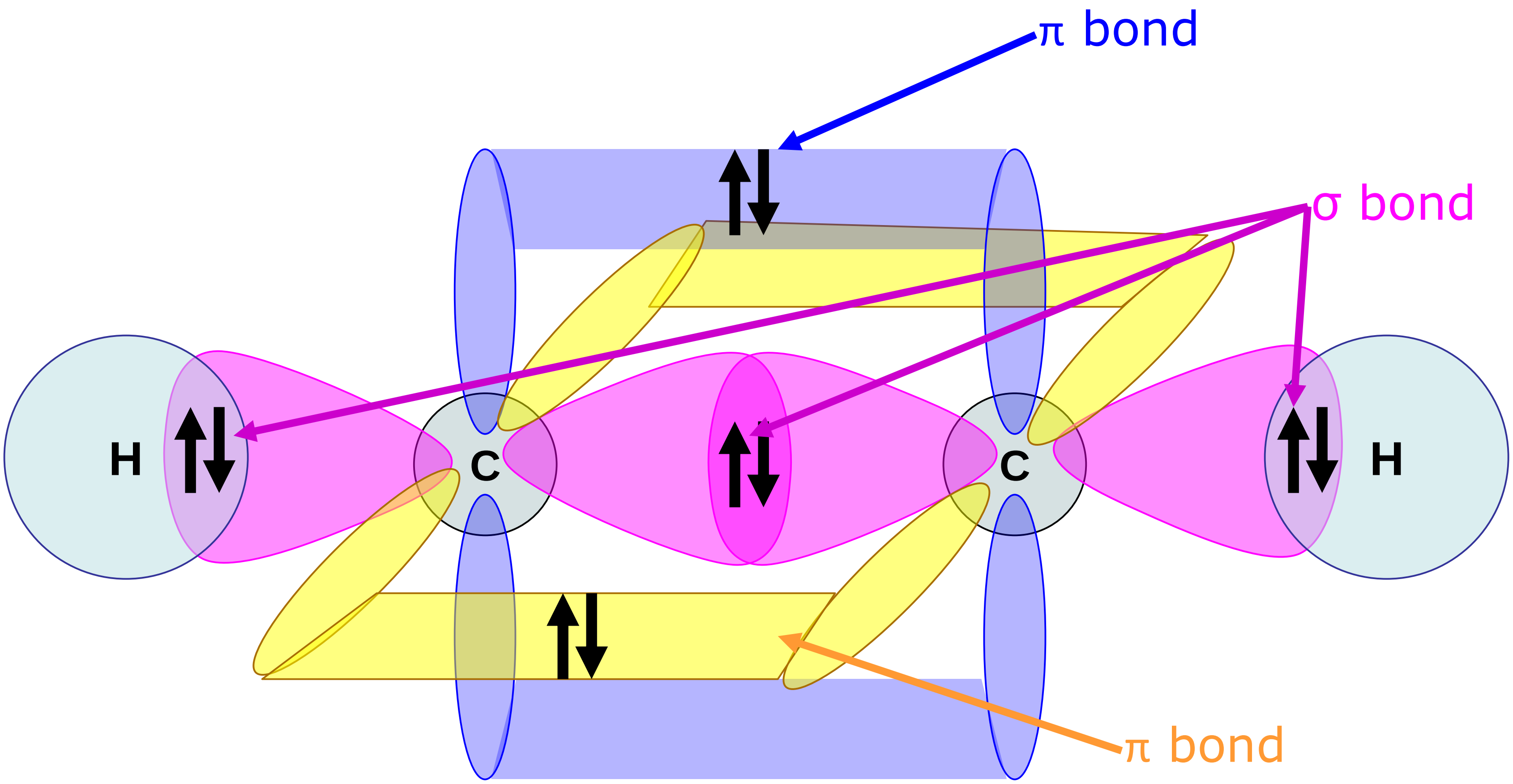
Example: C_2H_2

The orbitals will **hybridize** to make 2 sigma bonds + 2 pi bonds:



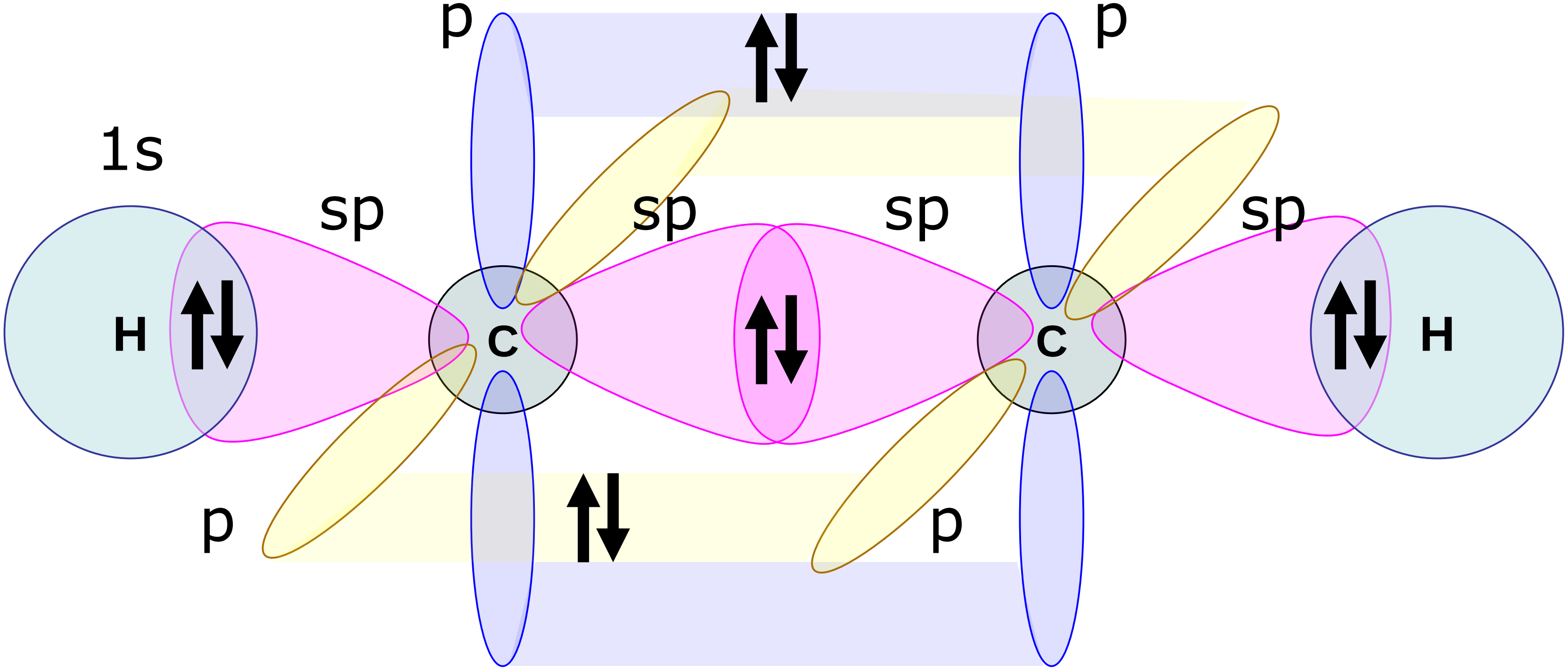
EXAMPLE: ETHYNE

Example: C_2H_2



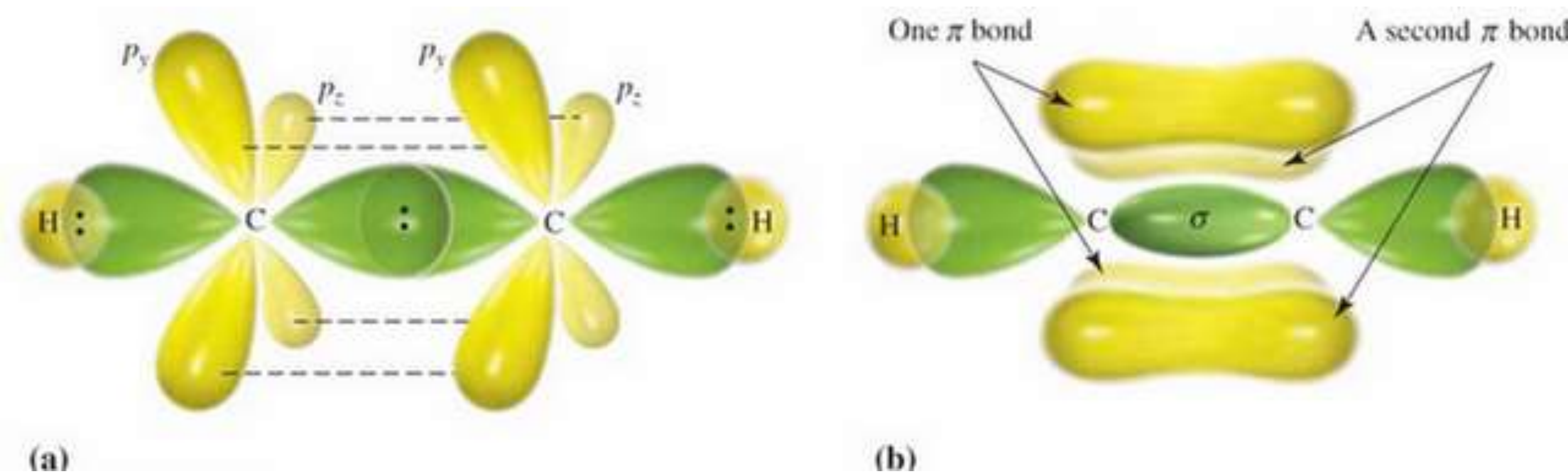
EXAMPLE: ETHYNE

Example: C_2H_2



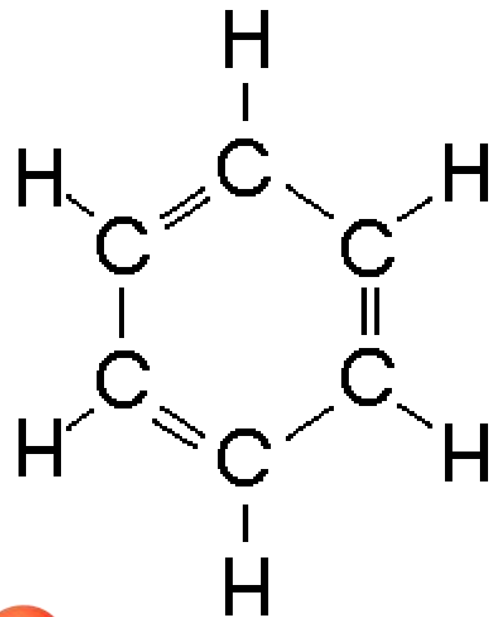
EXAMPLE: ETHYNE

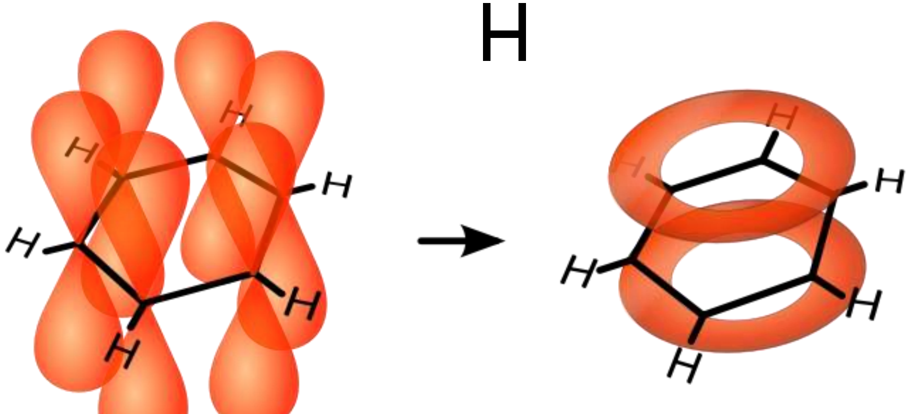
Example: C_2H_2



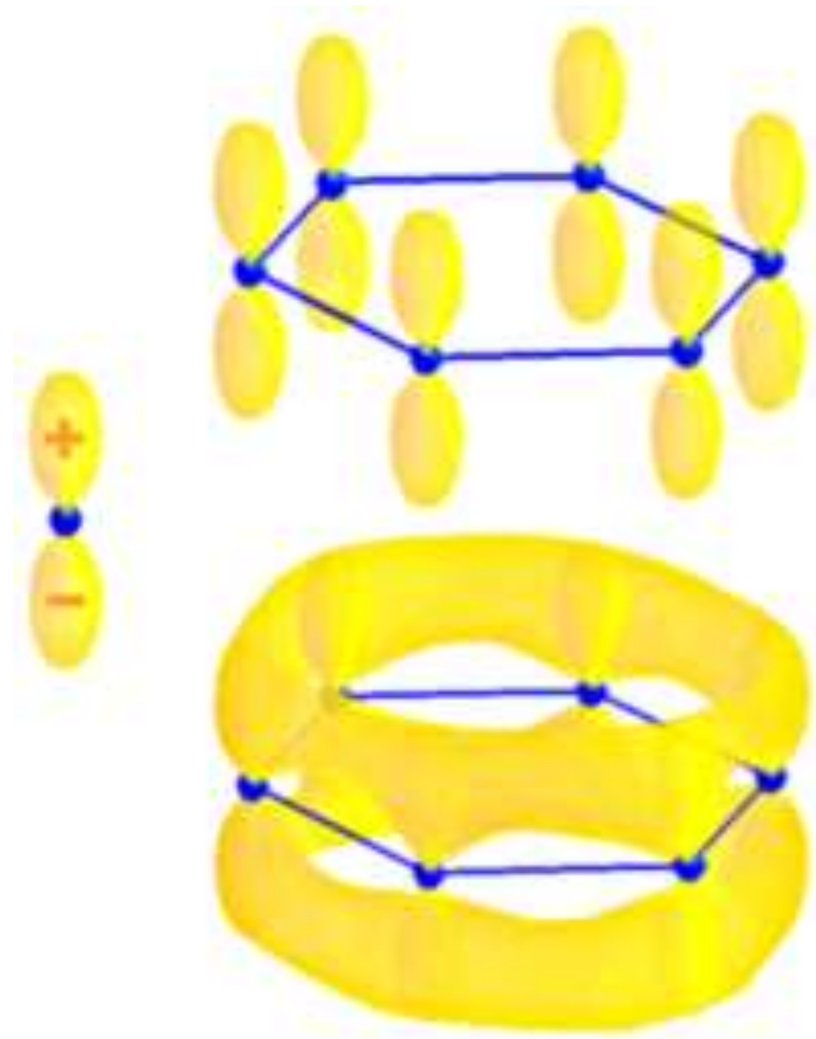
EXAMPLE: BENZENE

Example: C_6H_6





6 p-orbitals   delocalized



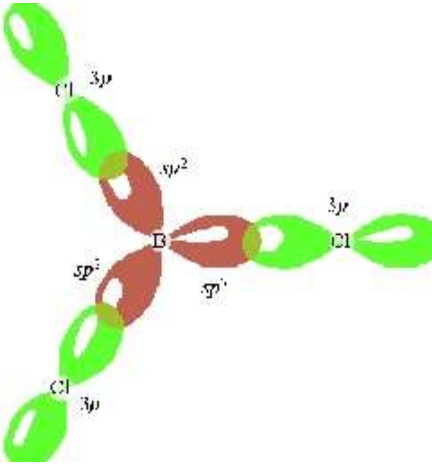
HYBRIDIZATION SUMMARY

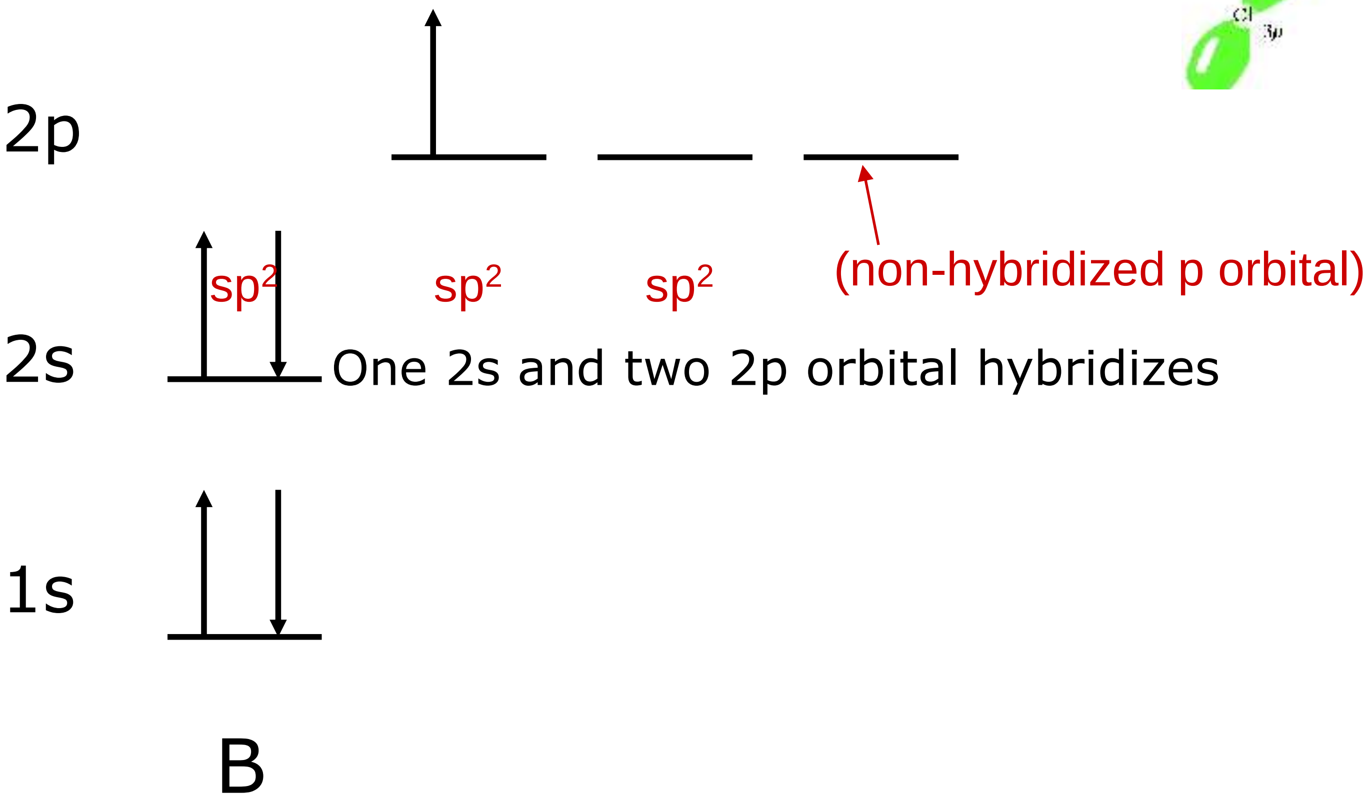
Summary: Hybridization of Carbon to Make Multiple Bonds

Bond Type	Hybrids	Pure	Bond Distribution
Single	4 sp^3	0	Hybrids make 4 σ bonds
Double	3 sp^2	1 p	π bond is made from pure orbital, σ is made from a hybrid
Triple	2 sp	2 p	π bonds are made from both pure orbitals, σ is made from a hybrid

HYBRIDIZATION OF BORON

Hybridization theory explains how **boron** can make 3 bonds (ex. BCl_3)





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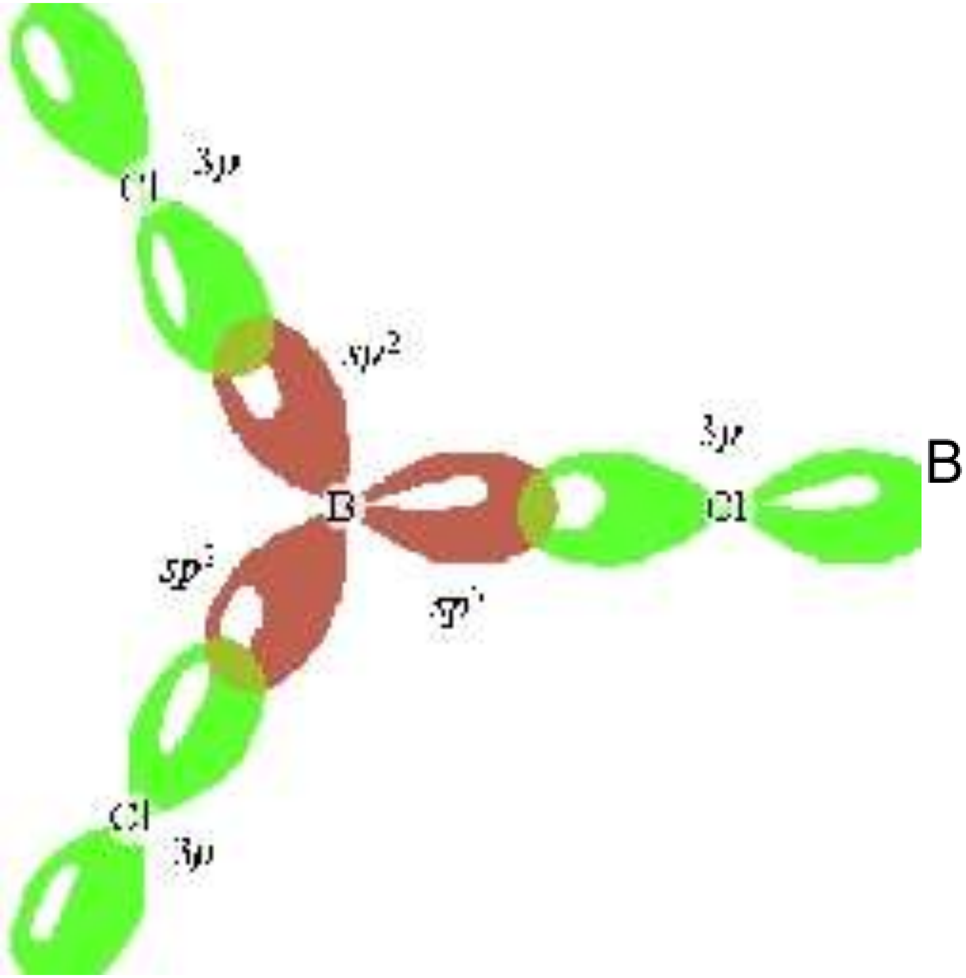
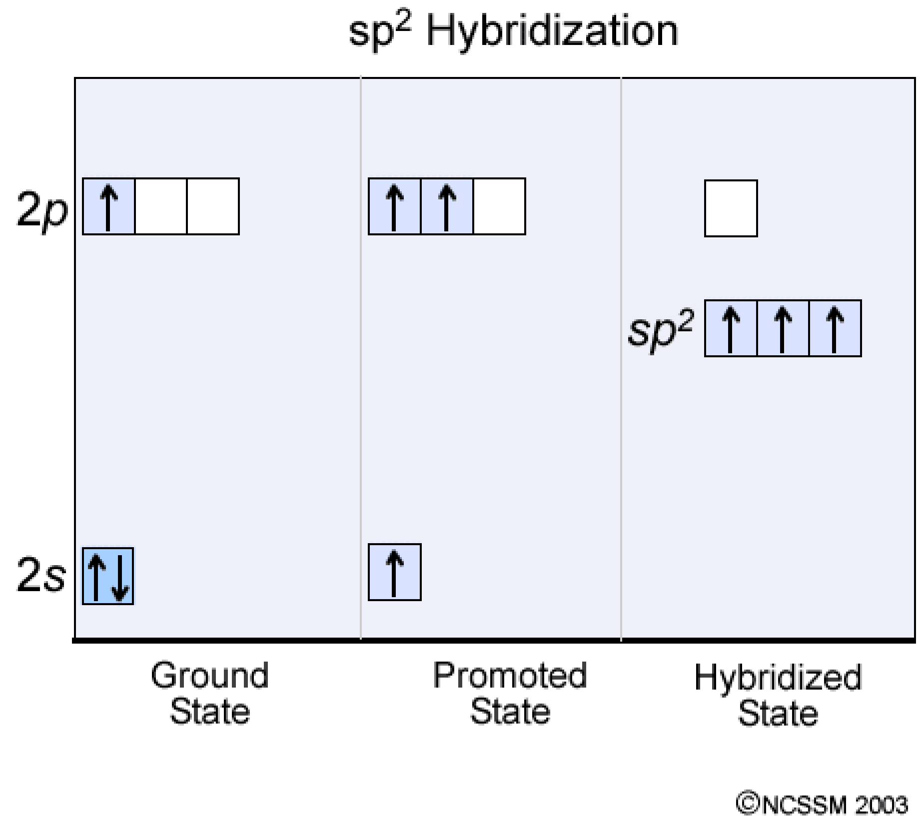
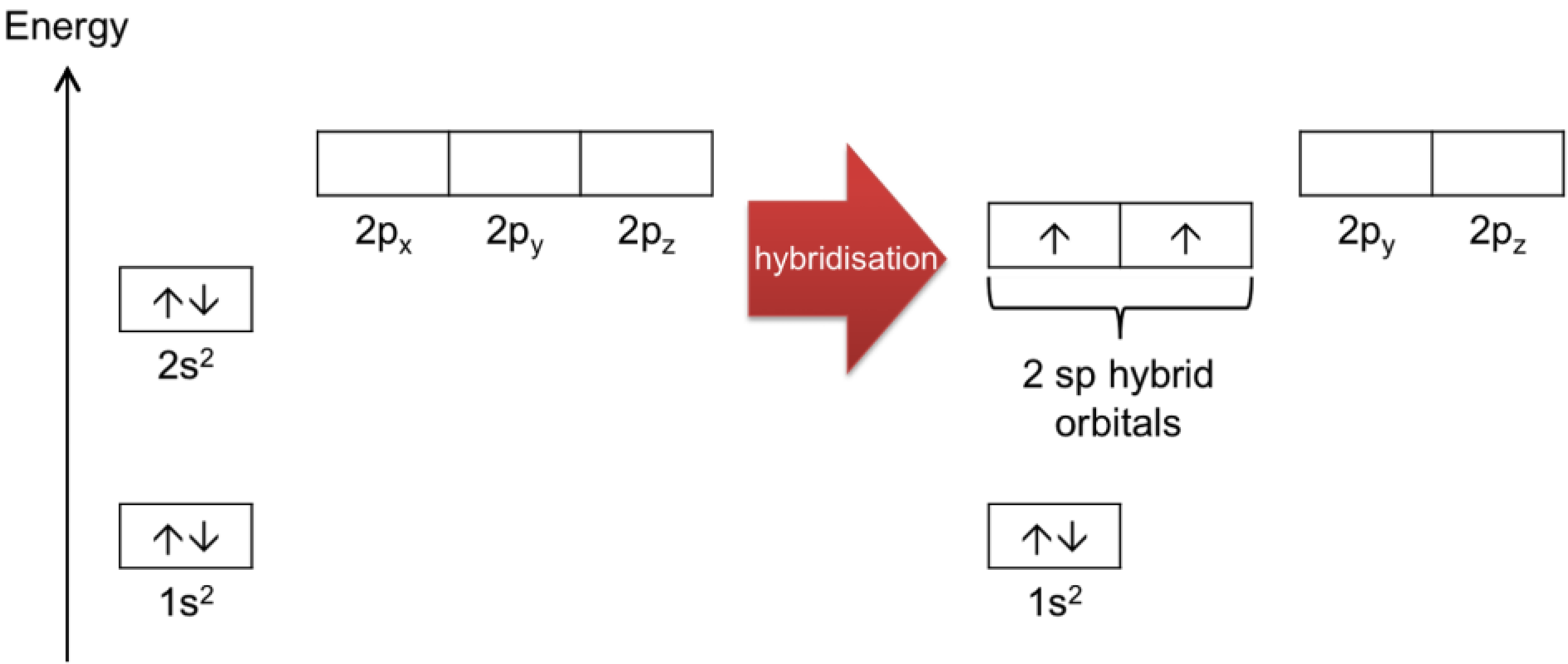




HYBRIDIZATION OF BERYLLIUM

Hybridization theory explains how **beryllium** can make 2 bonds even though its 2s orbital is full (ex. $BeCl_2$)



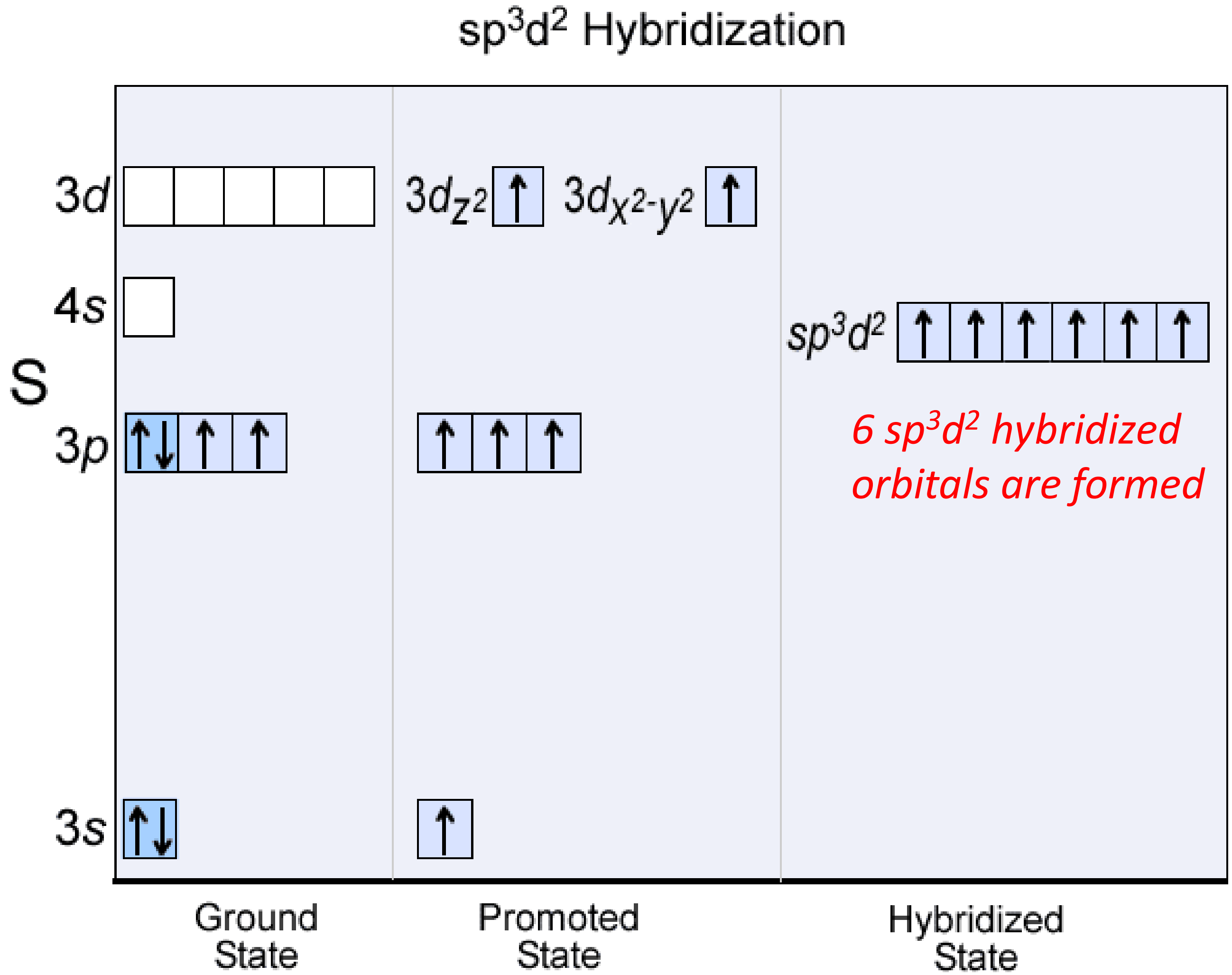
One electron from 2s is promoted to 2p to form two new hybridized orbitals

HYBRIDIZATION OF BERYLLIUM

Hybridization theory explains how **beryllium** can make 2 bonds even though its 2s orbital is full (ex. $BeCl_2$)

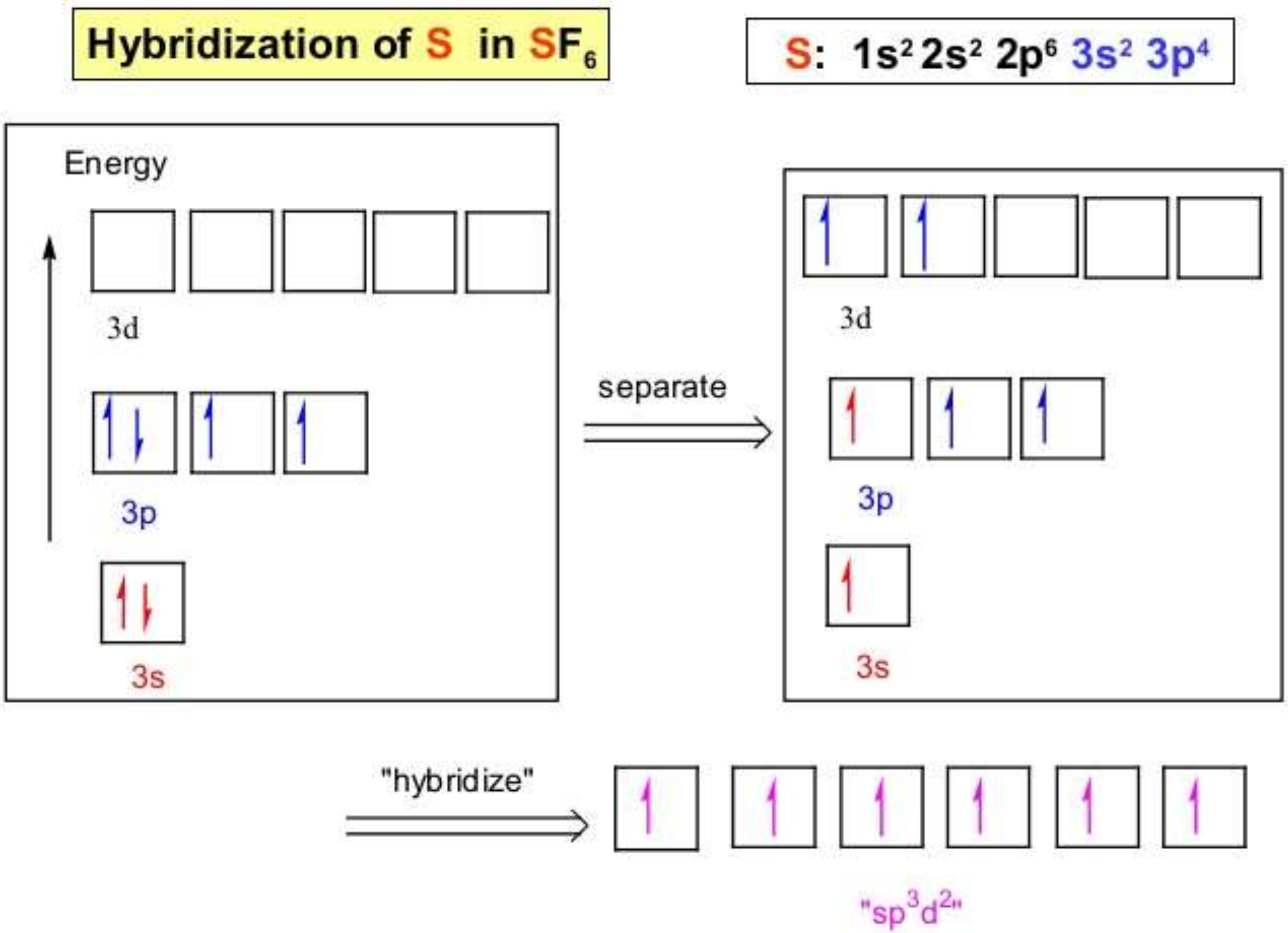
HYBRIDIZATION OF SULFUR

Hybridization theory explains how **sulfur** can make 6 bonds (ex. SF_6)



1 electron from 3s is promoted to 3p, and 2 electrons from 3p are promoted to 3d

HYBRIDIZATION OF SULFUR



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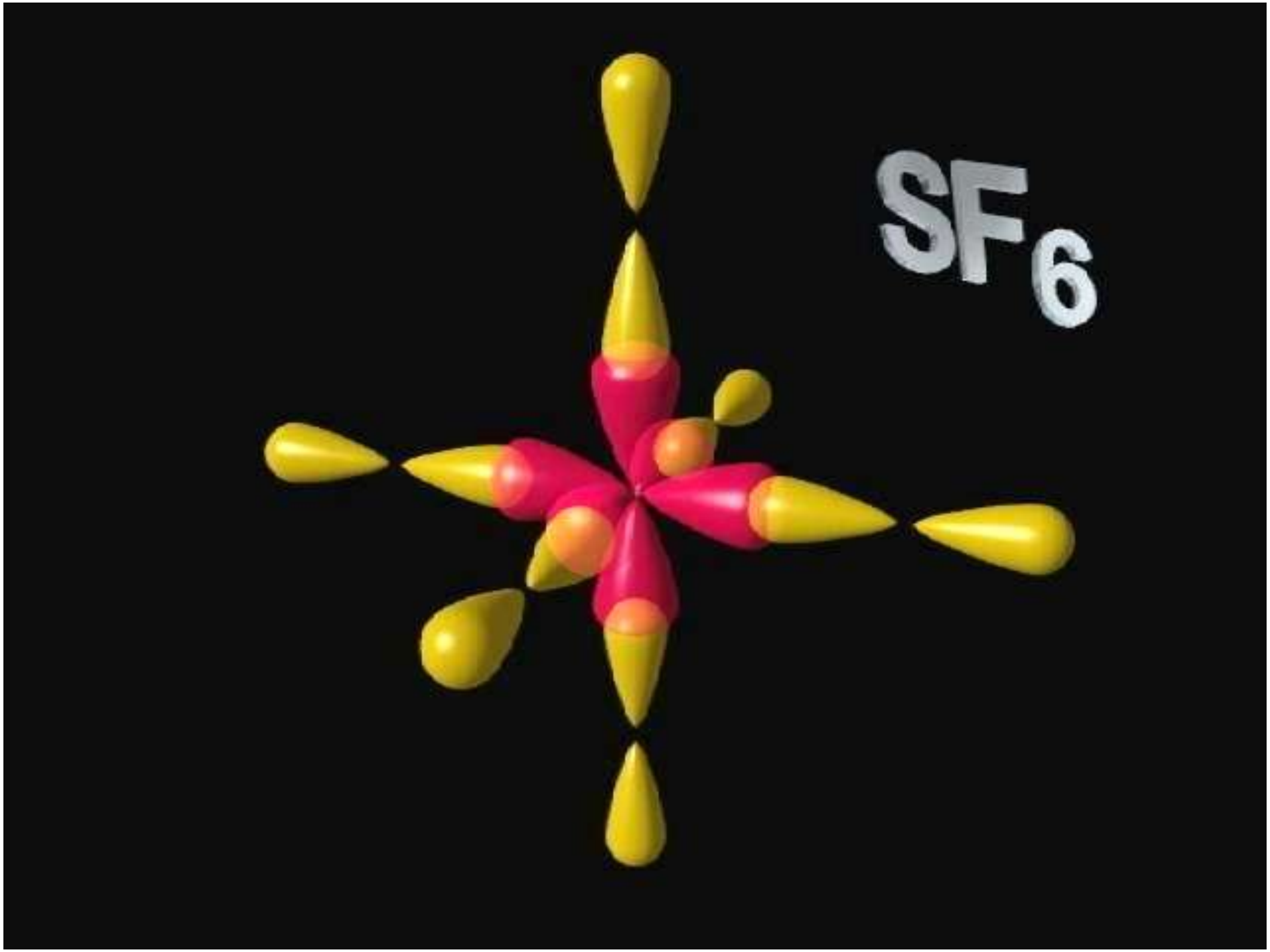
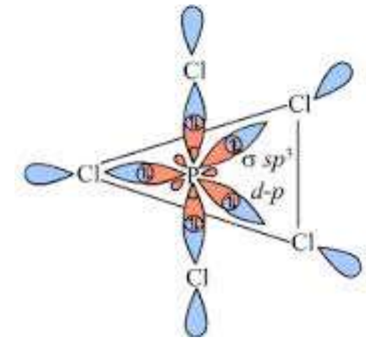


HYBRIDIZATION OF PHOSPHORUS

Hybridization theory explains how **phosphorus** can have a valence of +5 (ex. PCl_5)



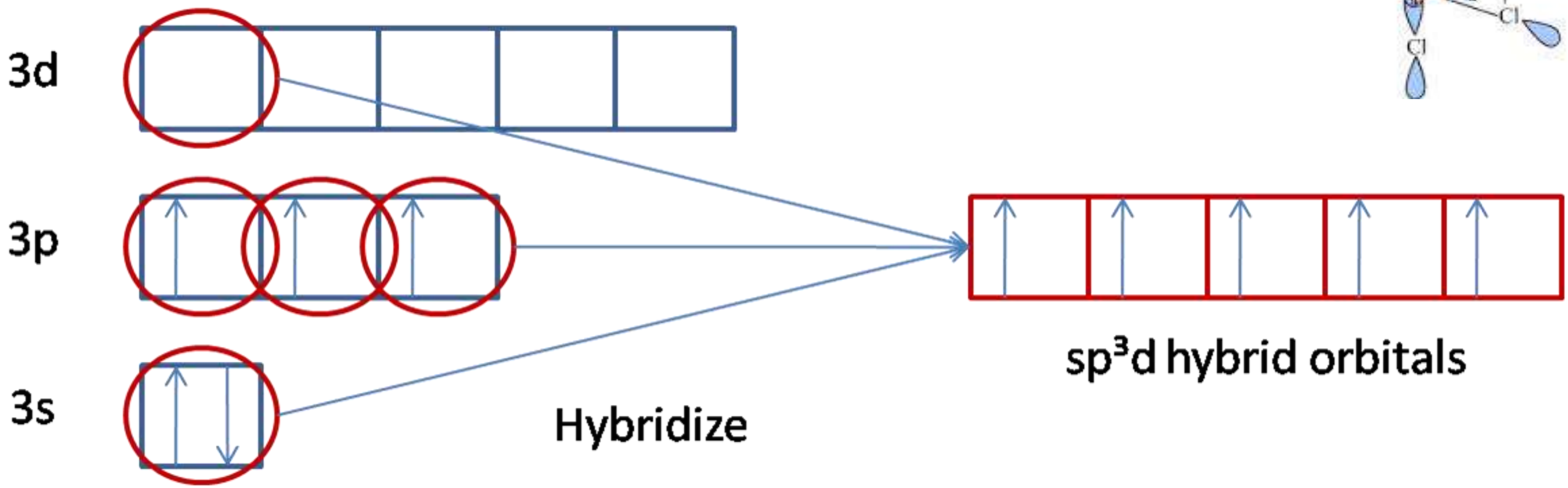


Figure1: Depiction of sp³d hybridization.

One 3s electron is promoted to 3d, forming 5 hybridized orbitals

HYBRIDIZATION OF PHOSPHORUS

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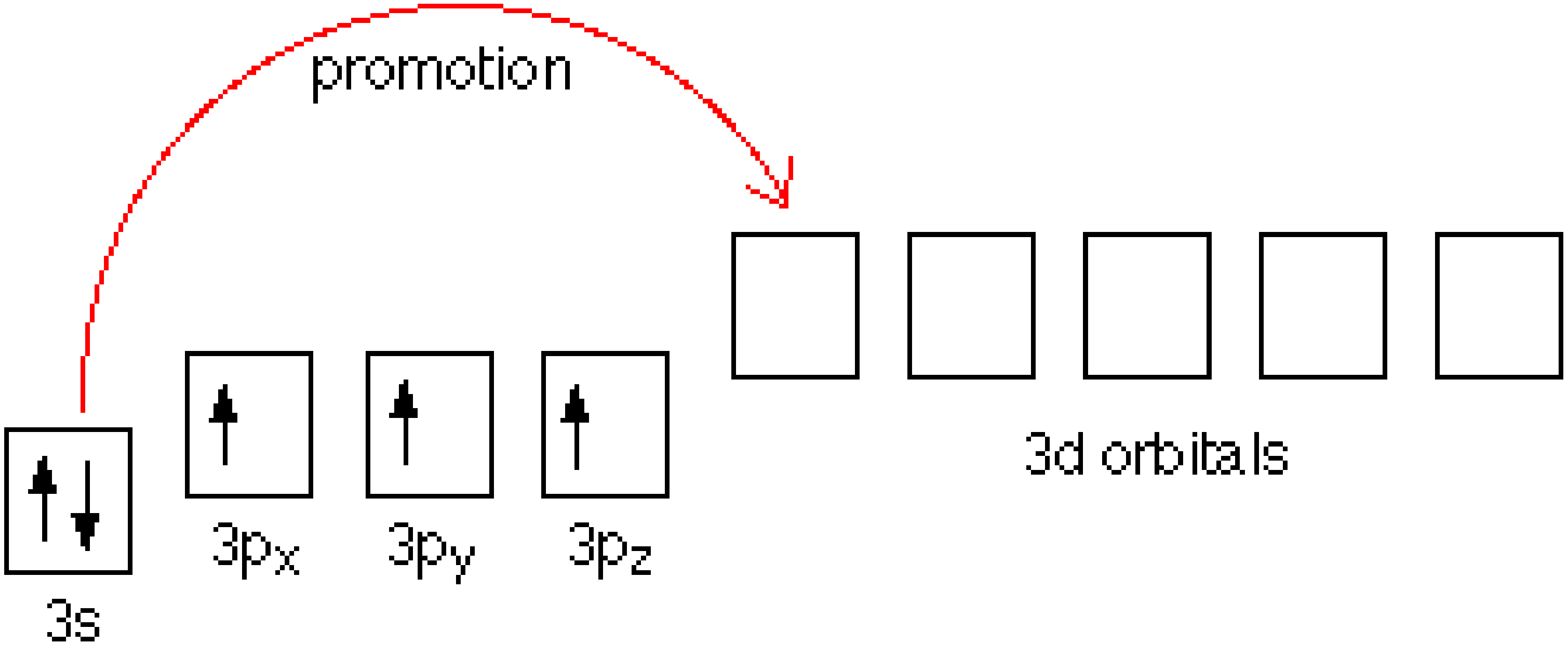

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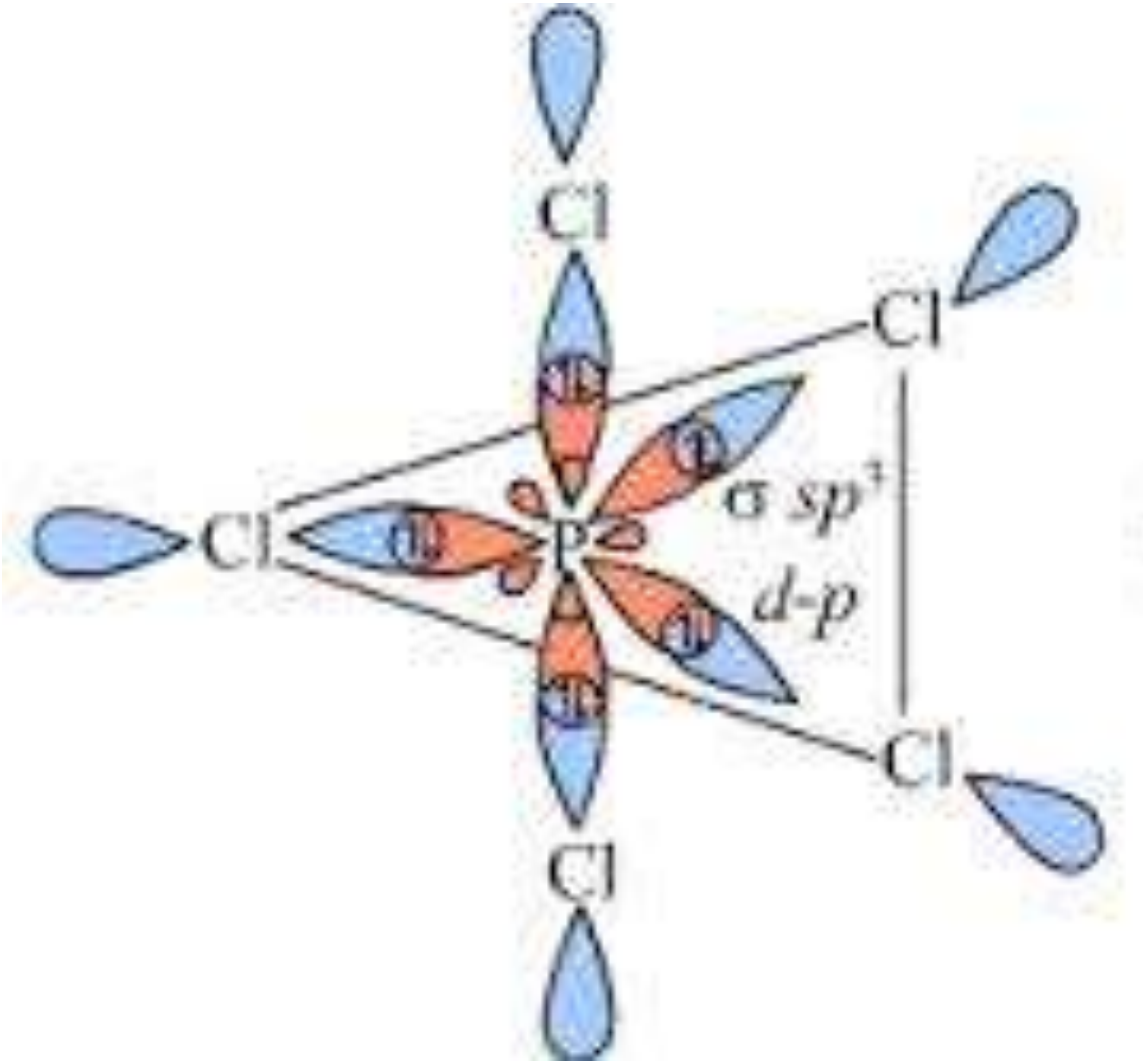

HYBRIDIZATION

Summary

Number of groups attached to central atom	Hybridization	Example
Two groups	sp	$BeCl_2$
Three groups	sp^2	BCl_3
Four groups	sp^3	CH_4
Five groups	sp^3d	PCl_5
Six groups	sp^3d^2	SF_6

HYBRIDIZATION

Homework

1. Use the valence bond model or hybridization theory to show the bonding in the following molecules: BeH_2, BH_3, CCl_4, PCl_5, SF_6

2. Page 238 # 1 – 5, 7, 8, 10