



# Molecular Orbitals

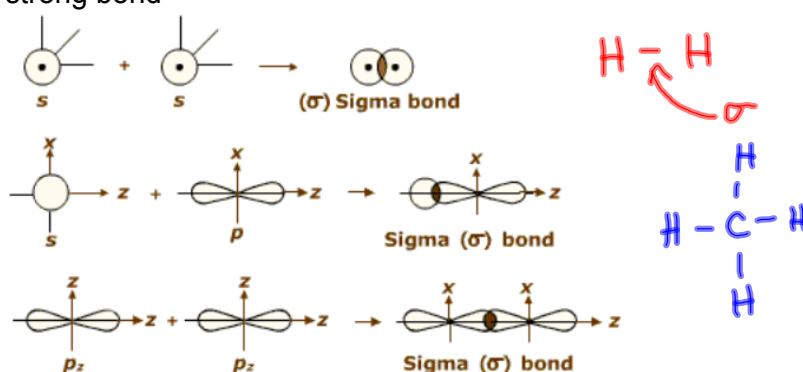
When two atoms share electrons to form a molecule, their atomic orbitals combine to produce molecular orbitals.

*s, p*

When the orbital is filled with two electrons, it is called a **bonding orbital**.

## Sigma bond

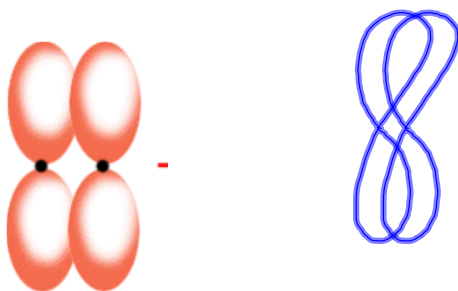
Bond that forms when two atomic orbitals overlap head-on.  
-strong bond



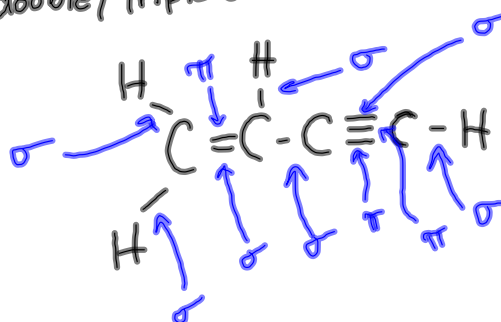
## Pi bond

*"p"*

Bond that forms when two atomic orbitals overlap side-by-side.  
-orbitals overlap less than in sigma bonds, thus the bonds are weaker than sigma bonds.



- double/triple bonds



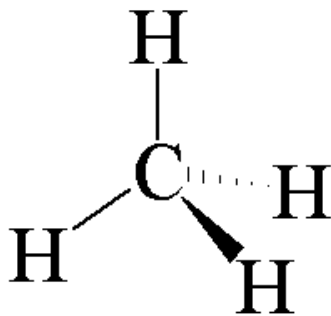


# VSEPR Theory

## Valence-Shell Electron-Pair Repulsion Theory

Repulsion between electron pairs causes molecular shapes to adjust so that the valence-electron pairs are as far apart as possible.

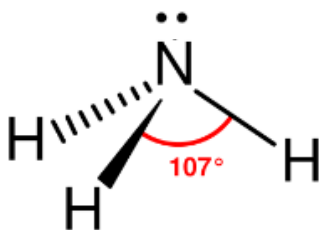
Ex.  $\text{CH}_4$



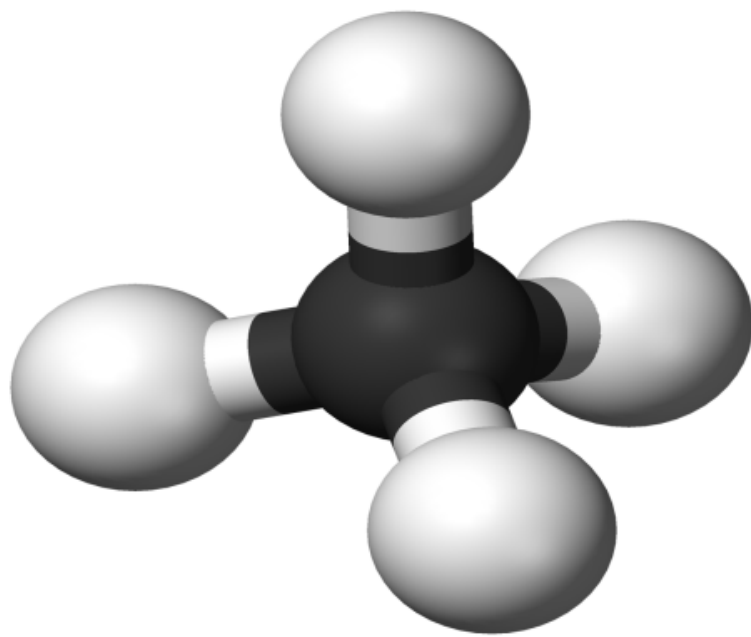
tetrahedral angle ( $109.5^\circ$ )

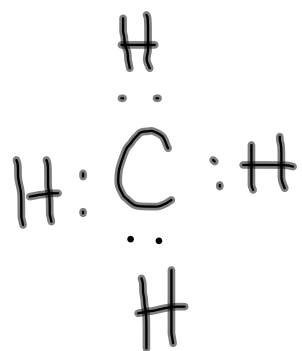
Ex.  $\text{NH}_3$

Lone pairs (unshared pairs) also affect the shapes of molecules.

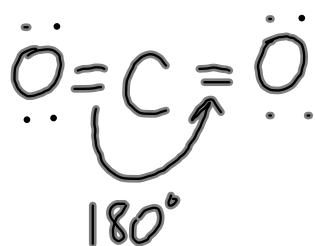


tetrahedral (pyramidal)





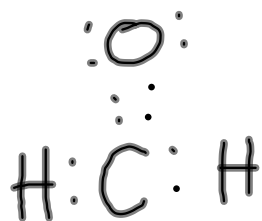
**Ex. CO<sub>2</sub>**



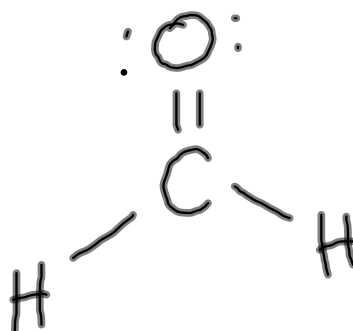
When predicting molecular shapes, double and triple bonds are treated as single bonds.

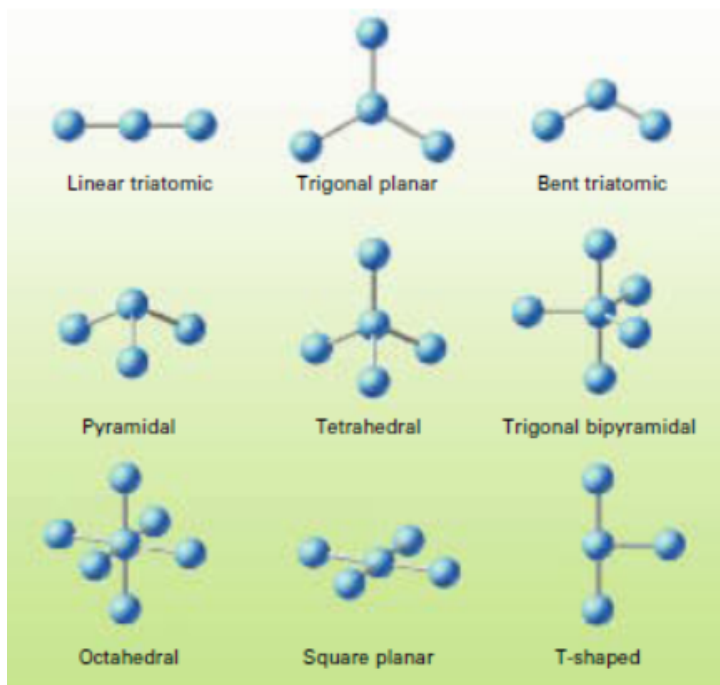
linear

**Ex. CH<sub>2</sub>O**



trigonal planar (120°)





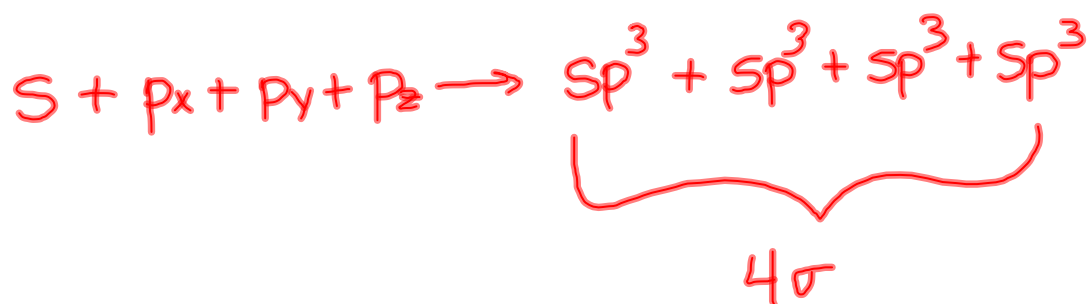
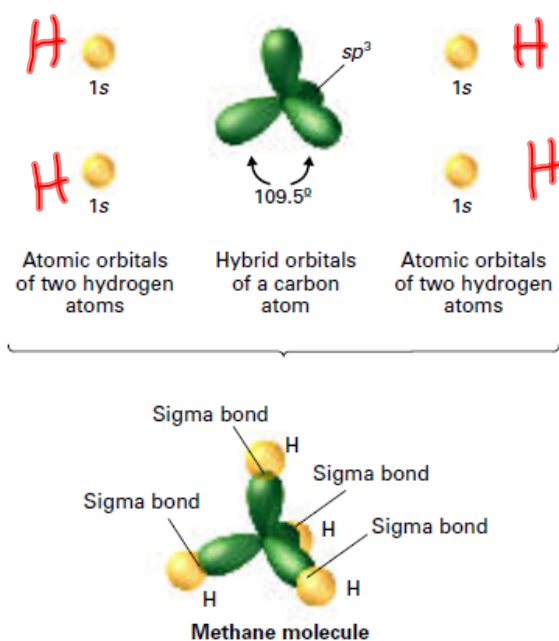


## Hybridization Involving Single Bonds

In <sup>S, P</sup>hybridization, atomic orbitals mix to form the same total number of equivalent hybrid orbitals.

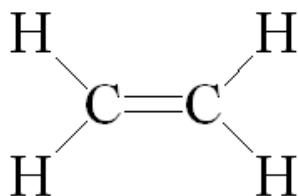
Ex. CH<sub>4</sub>

The one 2s orbital and three 2p orbitals of a carbon atom mix to form four sp<sup>3</sup> hybrid orbitals.



## Hybridization Involving Double Bonds

Ex.  $C_2H_4$

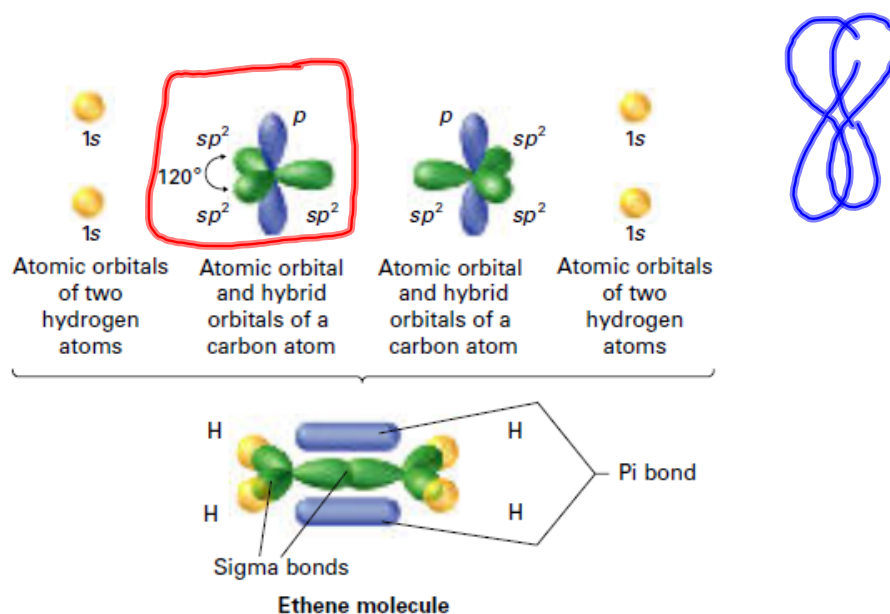


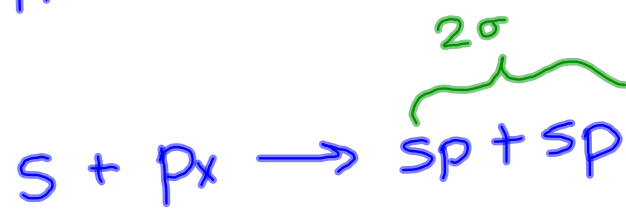
The one  $2s$  orbital and two  $2p$  orbitals of each carbon atom mix to form three  $sp^2$  hybrid orbitals.

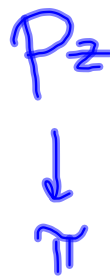
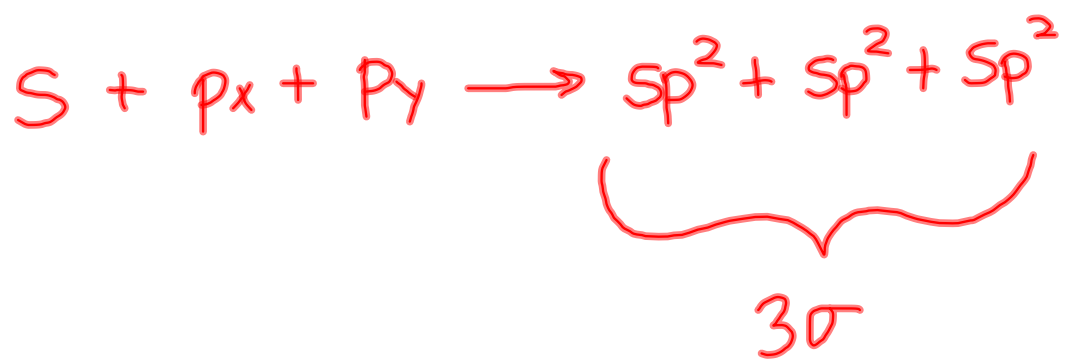
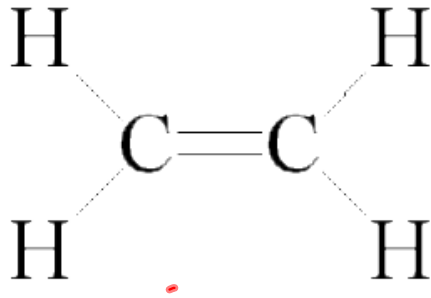
Two of the  $sp^2$  orbitals overlap with the  $1s$  hydrogen orbital to form carbon-hydrogen sigma bonds.

The third  $sp^2$  orbital overlaps with an  $sp^2$  orbital from the other carbon to form a carbon-carbon sigma bond.

The non-bonding  $2p$  orbitals overlap side-by-side to form a carbon-carbon pi bond.

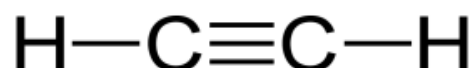






## Hybridization Involving Triple Bonds

Ex.  $C_2H_2$



The one  $2s$  orbital and one  $2p$  orbitals of each carbon atom mix to form two  $sp$  hybrid orbitals for each carbon.

One of the  $sp$  orbitals overlap with the  $1s$  hydrogen orbital to form carbon-hydrogen sigma bonds.

The second  $sp$  orbital overlaps with the  $sp$  orbital from the other carbon to form a carbon-carbon sigma bond.

The non-bonding  $2p$  orbitals overlap side-by-side to form two carbon-carbon pi bonds.

