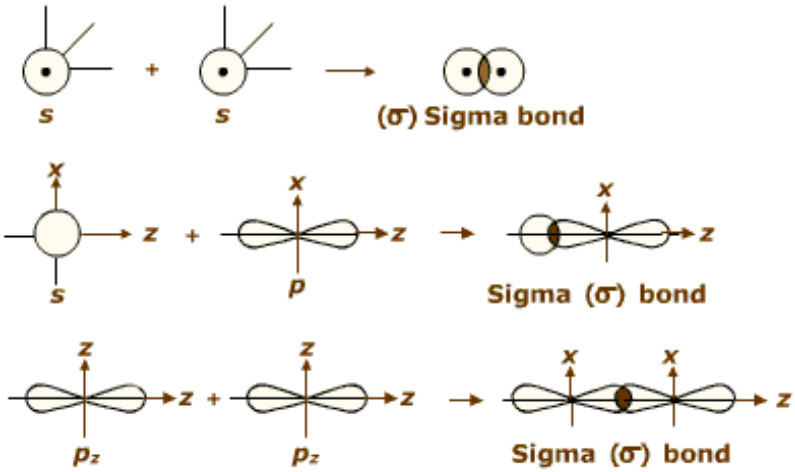
Molecular Orbitals

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

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

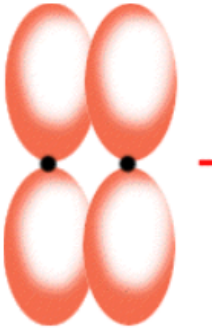
Sigma bond

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



Pi bond

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.

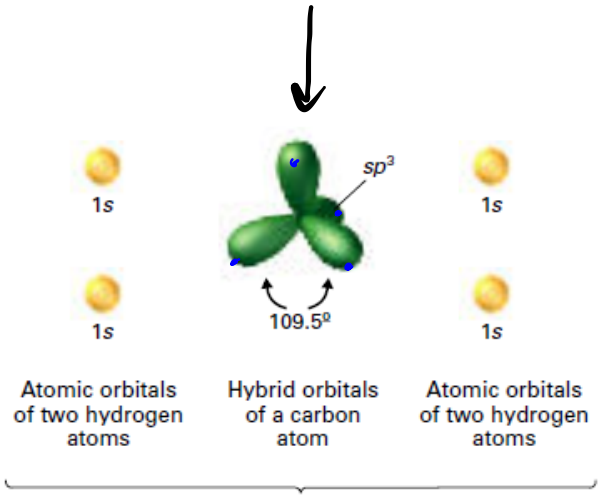


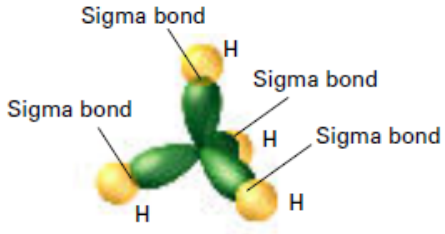
Hybridization Involving Single Bonds

In **hybridization** atomic orbitals mix to form the same total number of equivalent hybrid orbitals.

Ex. CH_4

The one *2s* orbital and three *2p* orbitals of a carbon atom mix to form four sp^3 hybrid orbitals.





Methane molecule

H 1s1

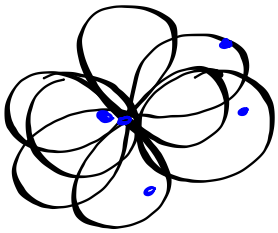
CH_4

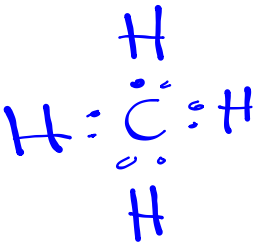
2p 1 1 1

2s 1

1s 11

C

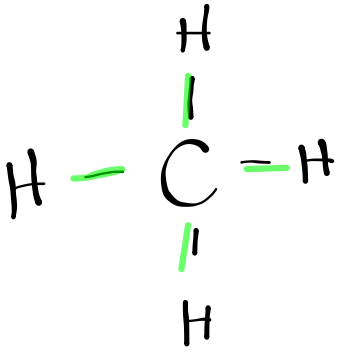




A.O. M.O.

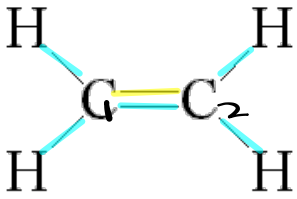
$S + p_x + p_y + p_z \longrightarrow sp^3 + sp^3 + sp^3 + sp^3$

40



Hybridization Involving Double Bonds

Ex. C_2H_4

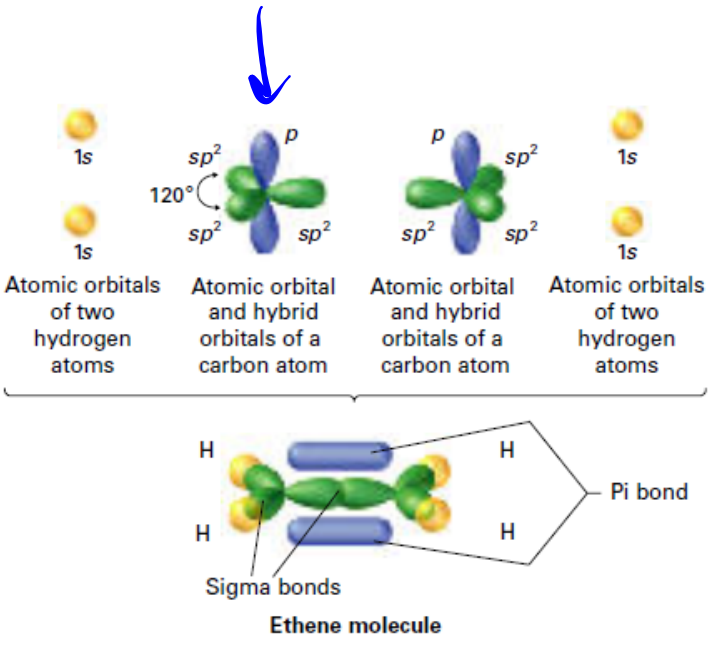


The one *2s* orbital and two *2p* orbitals of each carbon atom mix to form three sp^2 hybrid orbitals.

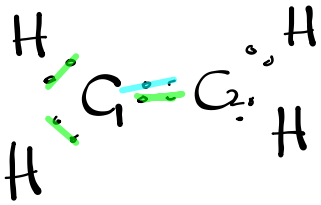
Two of the sp^2 orbitals overlap with the *1s* hydrogen orbital to form carbon-hydrogen sigma bonds.

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.



C_2H_4



$C_1 \rightarrow$ bonds to 3 atoms

↓

mix 3 orbitals

$s + p_x + p_z \longrightarrow sp^2 + sp^2 + sp^2$

3σ

$p_y \longrightarrow p_y \Rightarrow \pi$

Hybridization Involving Triple Bonds

Ex. C_2H_2

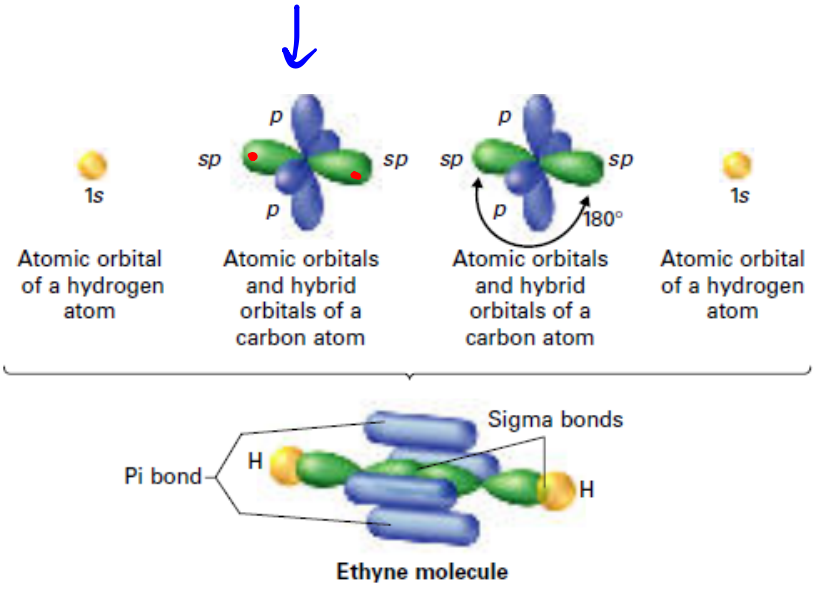
$$H—C\equiv C—H$$

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

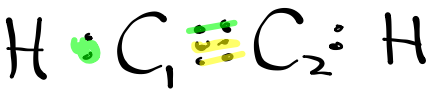
One of the *sp* orbitals overlap with the *1s* hydrogen orbital to form carbon-hydrogen sigma bonds.

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.



C_2H_2



C_1 → bonds to 2 atoms

↓

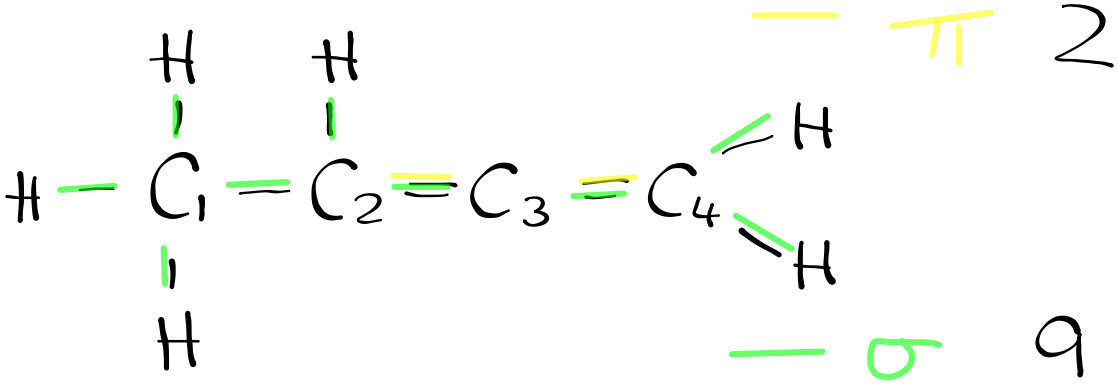
mix 2 orbitals

$S + p_y \longrightarrow$ sp + sp

2σ

p_x, p_z

2π



1. What type of hybrid orbitals used by each carbon?

C_1: $S + p_x + p_y + p_z \longrightarrow sp^3 + sp^3 + sp^3 + sp^3$ (4σ)

C_2: $S + p_x + p_y \longrightarrow sp^2 + sp^2 + sp^2$ $(3\sigma, 1\pi)$

C_3: $S + p_x \longrightarrow sp + sp$ $(2\sigma, 2\pi)$

C_4: $S + p_x + p_y \longrightarrow sp^2 + sp^2 + sp^2$ $(3\sigma, 1\pi)$

2. How many total sigma and pi bonds in molecule?

Homework

Worksheet