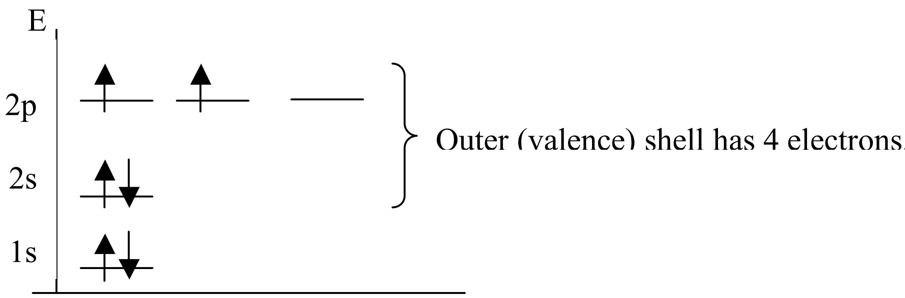
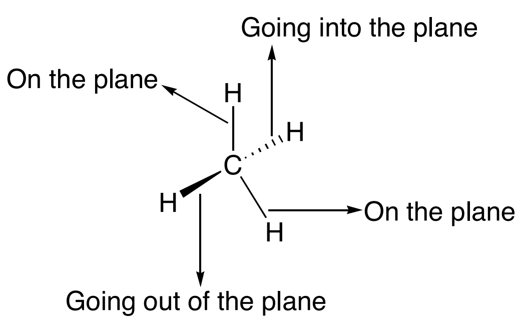
Carbon (C)



- For carbon to obtain inert gas configuration it can either give up 4 or gain 4 electrons.
- Since full loss or gain of electrons is unfavorable (would generate -4 or +4 charge), carbon shares 4 electrons to form "covalent bonds".

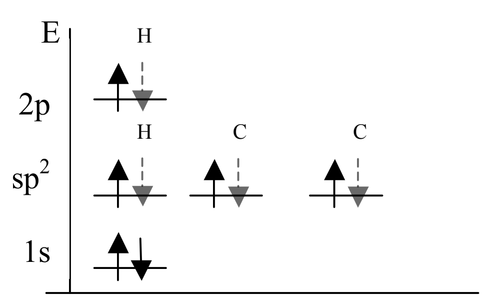
e.g. CH_4, methane



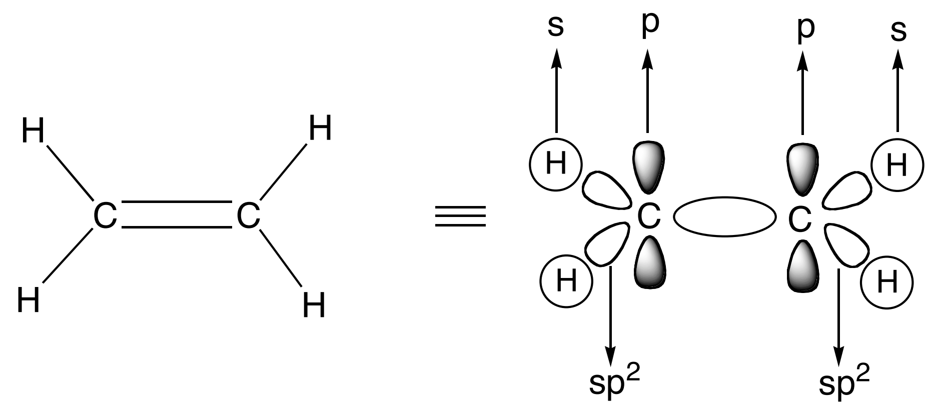
- Atomic orbitals of carbon are hybridized to give 4 sp^3 orbitals.
- Carbon is bonded with 4 H atoms (covalent bonds) wher each atom has the inert gas configuration

<u>sp^3 hybridization</u>
- Tetrahedral geometry
- Single bonds
- Bond angles of 109^o

<u>sp^2 hybridization</u>
- 3 atoms connected to carbon.
- Mixing of the 2s and two out of the three 2p orbitals. One p-orbital left over.
- Planar geometry
- Usually double bonds
- Bond angles of 120^o



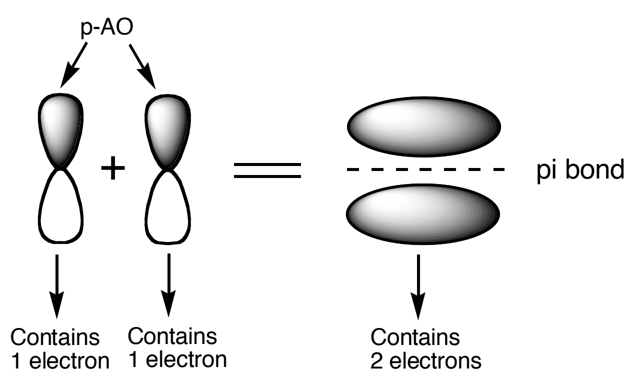
Ex) ethylene, ethene



- When atomic orbitals overlap they form molecular orbitals.
- Double bond contains one σ bond and one π bond.
- π bond fixes geometry, does not allow rotation along double bond.
- σ bond has free rotation.

<u>Linear Combination of Atomic Orbitals (LCAO)</u>

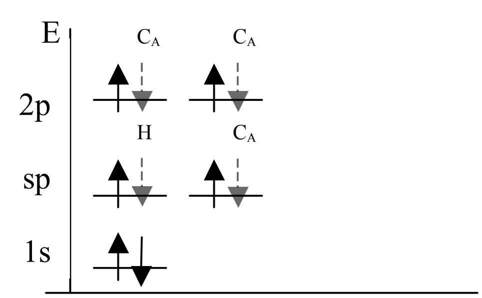
- Gives molecular orbitals (MO)
- Overlap of s atomic orbitals (AO) → gives sigma(σ) MO (cylindrical symmetry)
- Overlap of p AO → gives pi(π) MO



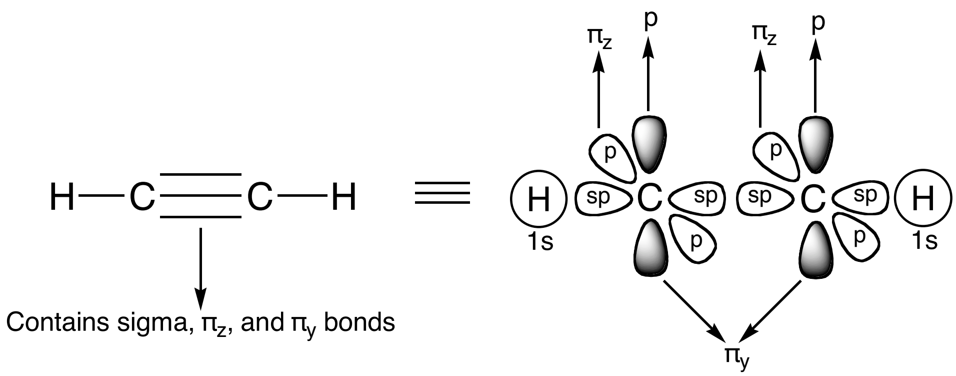
- Difference between AO and MO → AO present on an atom while MO present between two atoms when bond is formed.
- In terms of strength → σ bond is stronger than a π bond. But a double bond is stronger than a single bond because double bonds contain two bonds (σ-bond + π-bond).

<u>sp hybridization</u>

- Two atoms bonded to central atom
- Linear geometry
- Usually triple bonds
- Bond angle is 180°



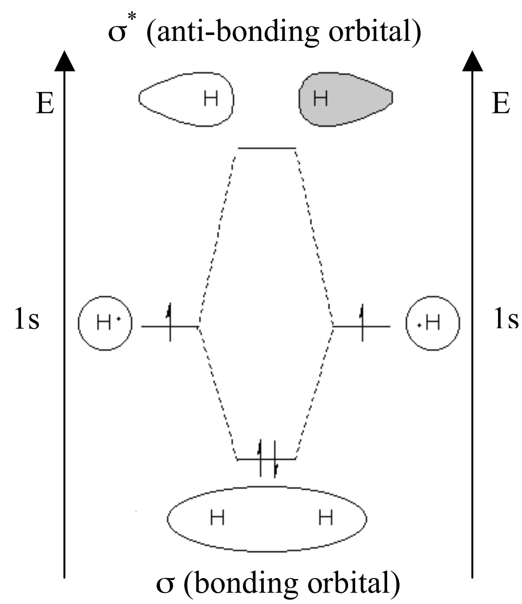
ex) Acetylene

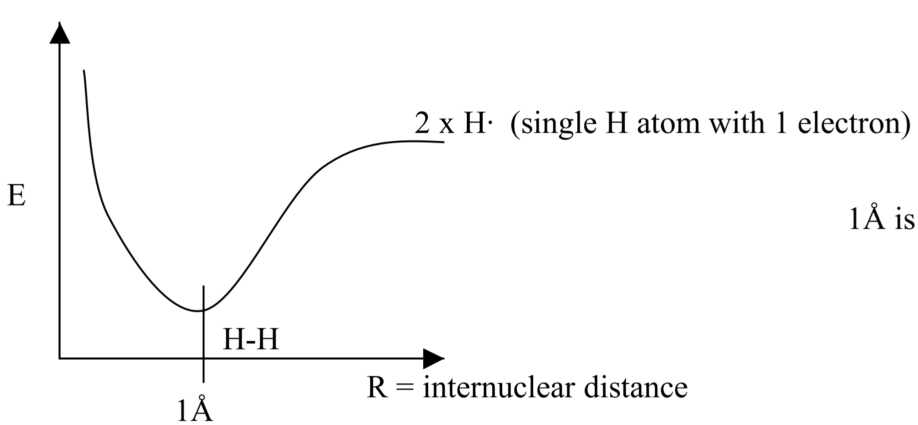


- Hybridization occurs in order to optimize geometry and decrease non-bonded interactions between atoms having inert gas configuration.

<u>Energetics of Forming Bonds</u>

ex) H_2





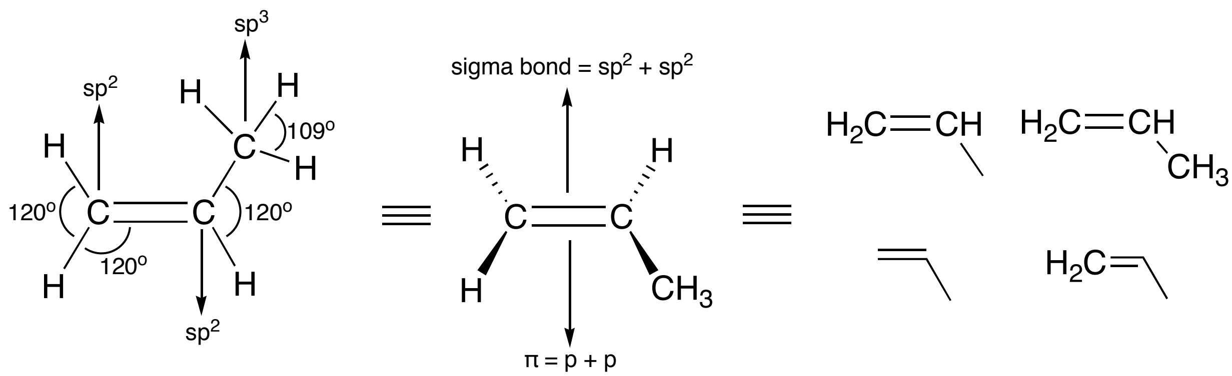
1Å is the average H-H bond distance

- Single bonds of H to C, O, N, F are ~1 Å = 10^{-8} cm
- Single bonds between C, N, or O are ~1.5 Å
- Double bonds between C, N, or O are ~1.35 Å
- Triple bonds between C, N, or O are ~1.2 Å

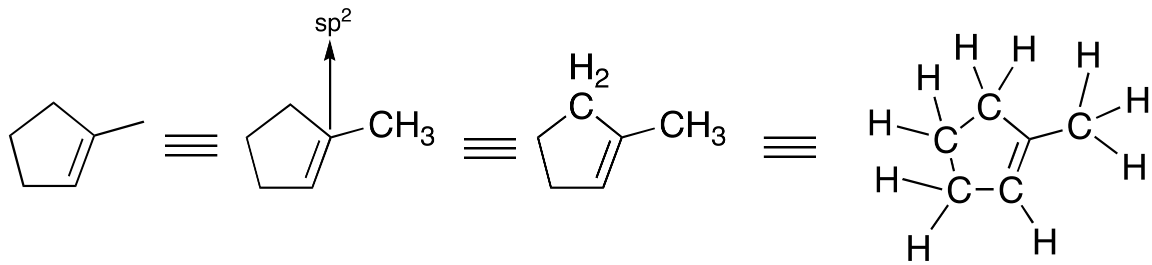
<u>Representation of Molecules</u>

- Show only electrons in outer (valence) shell
- Non-bonding electrons may not be shown
- Use element symbols, but carbon can be represented by point of angle or end of line
- Hydrogens and bonds to them from carbon are optional, show others

ex) C_3H_6 (propene)

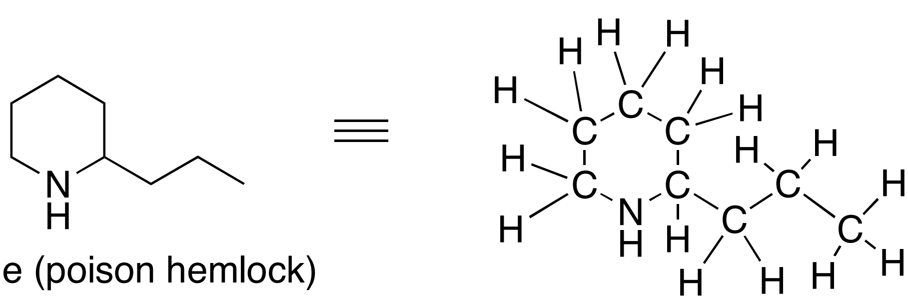


ex)



- ring strain can alter normal bond angles

ex)



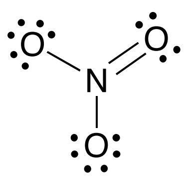
coniine (poison hemlock)

Formal Charge

- Convention to keep charges or know where they are
- ∑ (sum of) of formal charges = charge on molecule

Rules

- Add number of protons in nucleus
- Subtract number of inner shell electrons
- Subtract number of unshared electrons
- Subtract ½ of the number of shared outer shell electrons

ex) 

Nitrate

Formal charge on N = +7

-2 (1s electron)

0 (unshared electrons)

(1/2 x 8) = -4 (1/2 unshared electrons)

+1