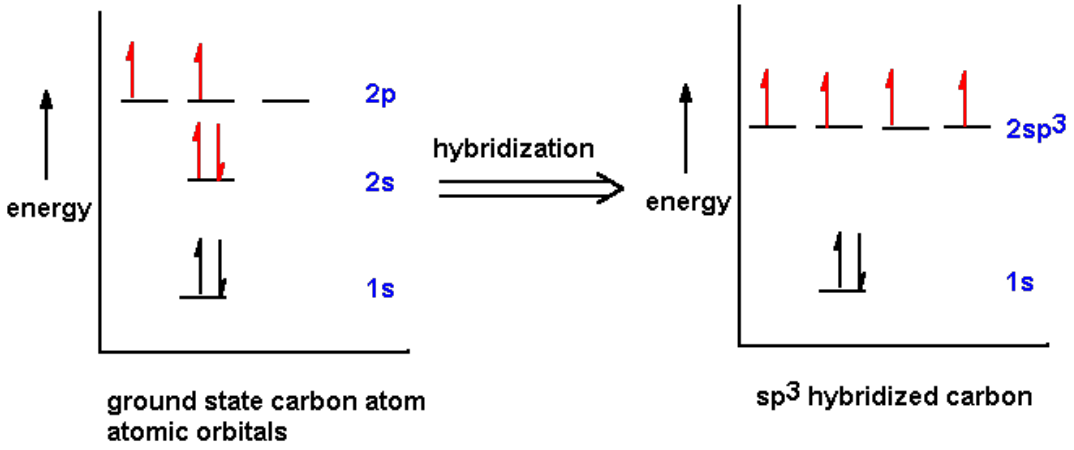
**Hybridization:**

- Mixing of atomic orbitals (with the wrong geometry for bonding) to form hybrid orbitals with the correct geometry for bonding
- Will only happen for bonding

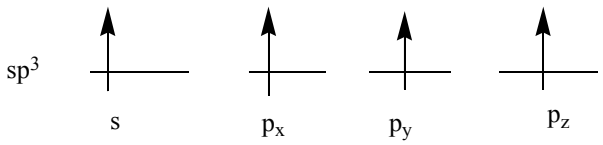
**LCAO**

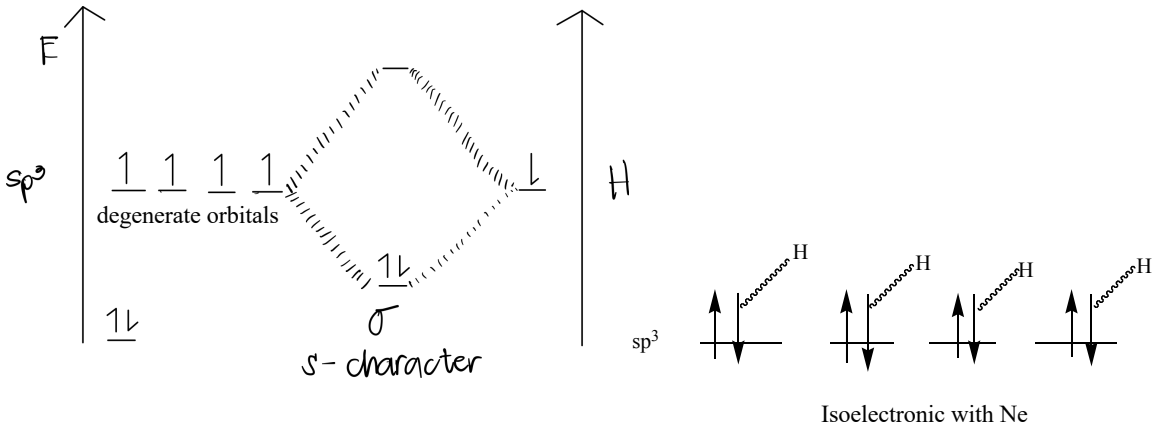
- Linear combination of atomic orbitals (LCAO)
- Combination of atomic orbitals of s- character gives molecular orbital called sigma molecular orbital (σ)




**$sp^3$ Hybridization**

- Single bonds in 2nd row elements
- Tetrahedral geometry
- Angle between two H atoms in methane: 109°, close to that with other elements
- Often free rotation around single bonds
- $sp^3$ orbitals are lower in energy then the respective p orbitals of carbon
- Overlap of atomic orbitals with s component gives sigma molecular orbital (bond)
- Each line in a structure represents 2 $e^-$
- All atoms want to be electronically stable
- All atoms want to be isoelectronic with a noble gas
  H → He ; C → Ne
- C-H bond → $sp^2$ + s
- C = C → one is $sp^2$ + $sp^2$ and one is p + p





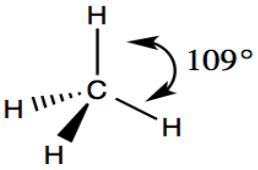

Isoelectronic with Ne

**sp² Hybridization**

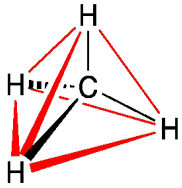
- Double bonds in the 2nd row
- Three things bonded to 2nd row atom
- Planar geometry
- Angle between two atoms: 120°
- No free rotation around double bonds because the p orbitals have to line up
- Overlap of atomic orbitals with s component gives sigma molecular orbital (bond)
- Overlap of p atomic orbitals with p component gives pi molecular orbital (bond)

**Drawing Molecules**

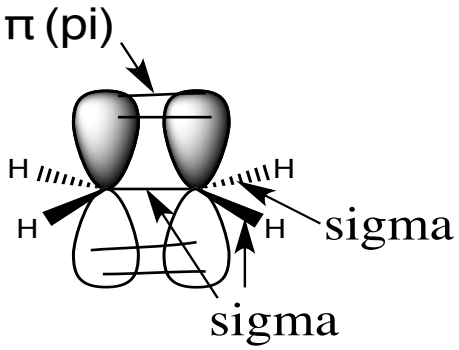
- Solid wedge ( ): Toward you / out of the page
- Dashed wedge ( ): Away from you / into the page
- Plain solid line ( ) : undefined geometry or in-plane

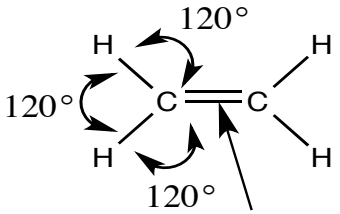



$CH_4$ - Methane




The red lines outline a tetrahedron
Black lines show the covalent bonds

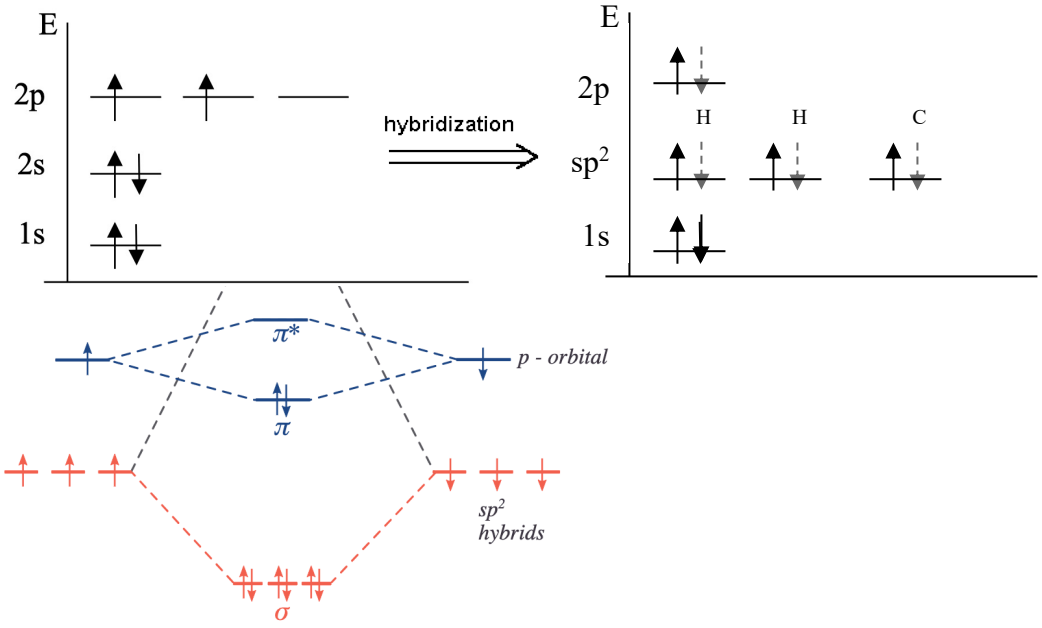


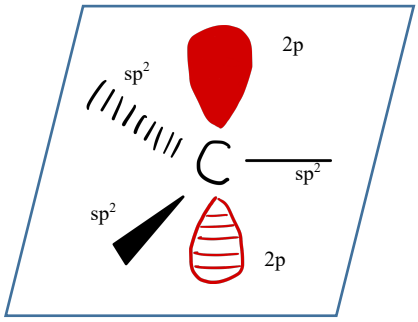

ethylene = ethene

sigma + pi = double bond

$sp^2$+$sp^2$ p+p




*only depicting valence shell electrons (1s typically not included)

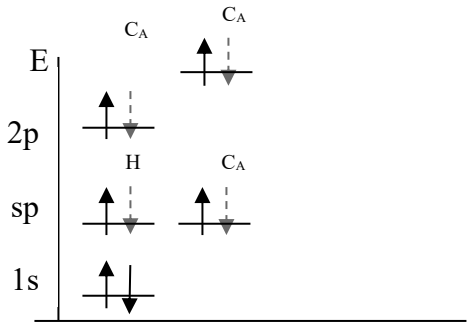



p + p → π molecular orbital

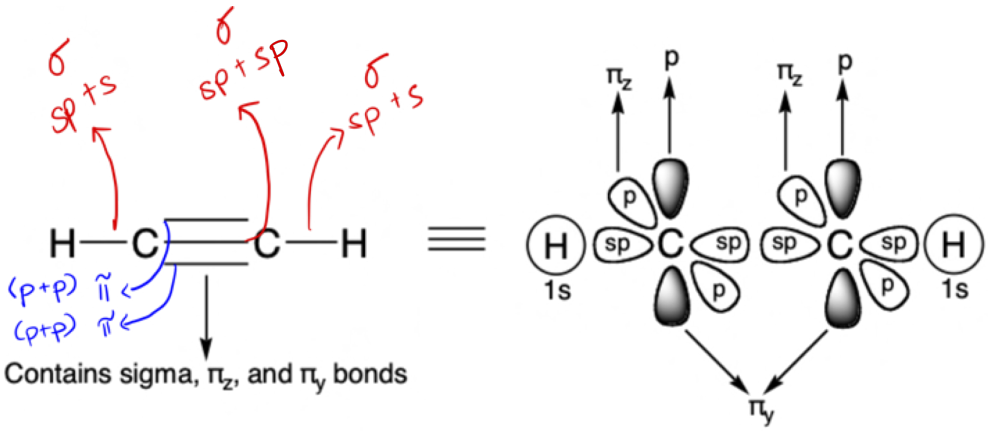
- $sp^2$ carbon is in planar geometry; all atoms are in planar

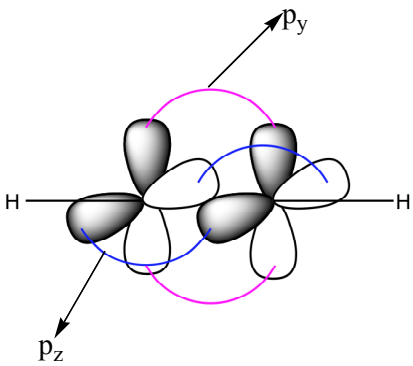
## sp Hybridization

- Triple bonds
- Two atoms bonded to C
- Linear geometry
- One sigma bond and two pi bonds
- No free rotation around triple bonds
- Angle between two atoms: 180°



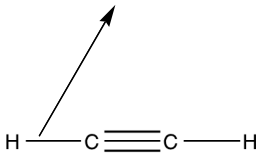

**e.g. Acetylene/Ethyne**




**Triple bond:**
One sigma bond between the carbons plus two pi bonds formed through $p_y$ and $p_z$

sigma (s of H and sp of C)

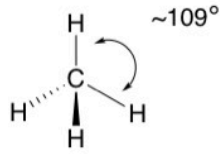



acetylene = ethyne

**Hybridization ($sp^3$ vs $sp^2$)**

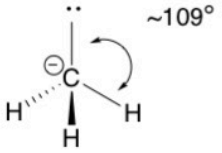
- $Sp^3$ hybridized atoms have 4 "things" attached and has a tetrahedral geometry (108.5° bond angles)
- $Sp^2$ hybridized atoms have 3 "things" attached and has a planar geometry (120° bond angles)

Methane ($CH_4$)



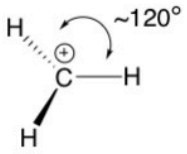

$sp^3$ hybridization

Methyl Anion ($CH_3^-$)



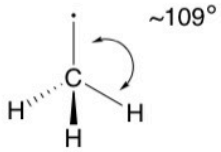

$sp^3$ hybridization

Methyl Cation ($CH_3^+$)



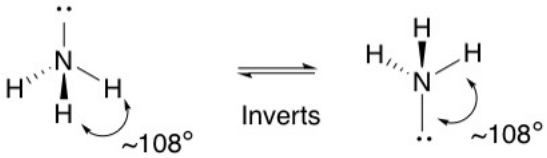

$sp^2$ hybridization

Methyl Radical ($CH_3\bullet$)



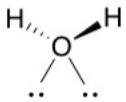

$sp^3$ hybridization

Ammonia

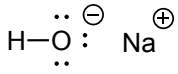



$sp^3$ hybridization

Water



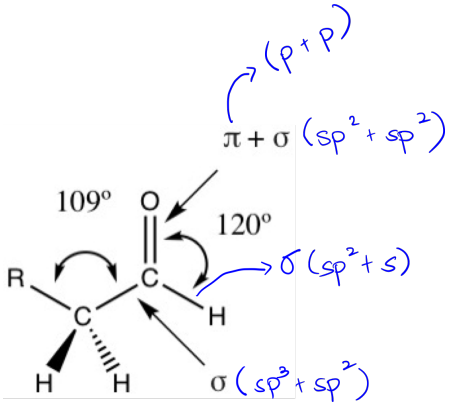
$sp^3$ hybridization




$sp^3$ hybridization

**`Hybridization ($sp^3$ vs $sp^2$) cont.**

Overlap of p orbitals to form pi (π) bonds precents free rotation around double bonds
**e.g. Aldehyde**




R= any group

The $CH_2$ is $sp^3$ hybridized, the atoms attached to it have a bond angle of 109°
The carbonyl carbon is $sp^2$ hybridized, the atoms attached to it have a bond angle of 120°

The oxygen contains two lone pairs (not drawn), it is $sp^2$ hybridized
The single C-C bond can freely rotate.

**Size and Shape of Molecules: determined by bond lengths and bonding type**

- Geometry is dictated based on filled orbitals moving as far apart as possible
- A bond length between hydrogen and a 2nd row element is approximately 1A

NOTE THE FOLLOWING (Estimated bond length between atoms)


1Å 1.5Å 1.35Å 1.25Å

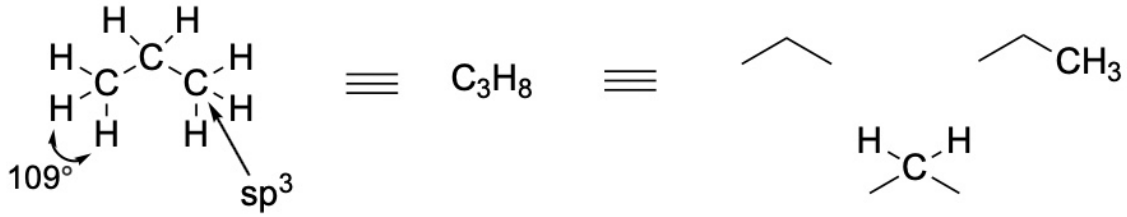
X = C, O, N

**<u>Representation of Molecules</u>**

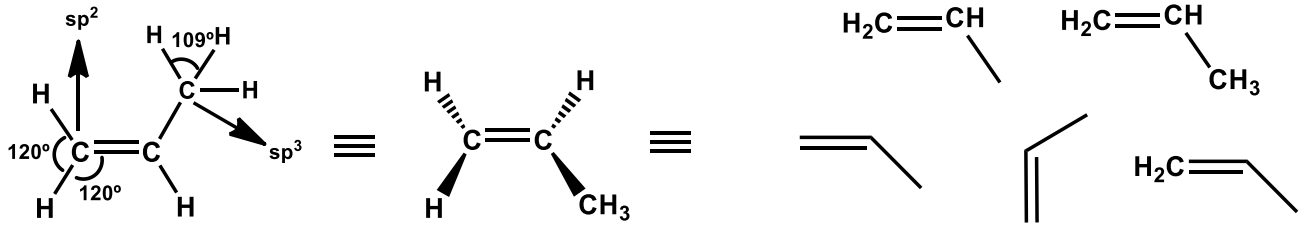
- Show only electrons in outer (valence) shell
- Line represents two bonded electrons`
- Non-bonding electrons (lone pairs) may or may not be shown
- Use element symbols, but carbon can be represented by point of angle or end of line
- Hydrogens and bonds to them from carbon are optional; show others.
- Each line in a structure represents 2 $e^-$
- Solid wedge ( ◥ ): Toward you / out of the page
- Dashed wedge ( ⋯⋯ ): Away from you / into the page
- Solid line (——— ): undefined geometry or in-plane

**Examples:**

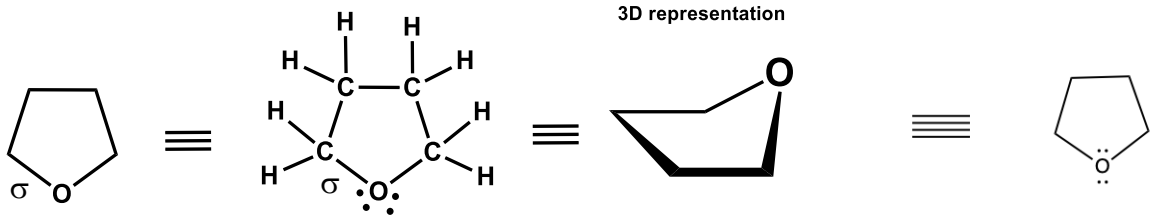
1. **Propane ($C_3H_8$):**




2. **Propene ($CH_3CHCH_2$):**



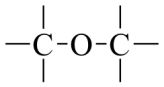

### 3. Tetrahydrofuran (THF)




Chemical Formula: $C_4H_8O$
Molecular Weight: 72.11

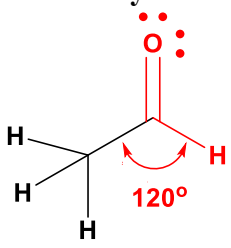
**Oxygen in the stable uncharged state forms two bonds with 2 lone pairs of electrons**
**Nitrogen in the stable uncharged state forms three bonds with 1 lone pair of electrons**

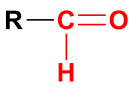
NB: Functional Group in Tetrahydrofuran is ETHER

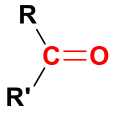



ETHER

### 4. Aldehyde and carbonyl

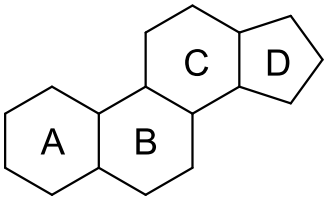



**Acetaldehyde** **Aldehyde** **Carbonyl**

**5. Steroid Molecule**

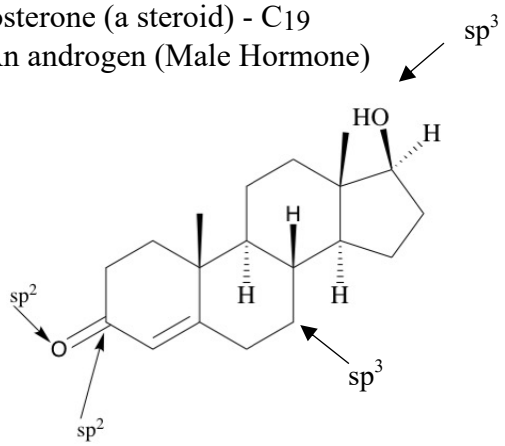


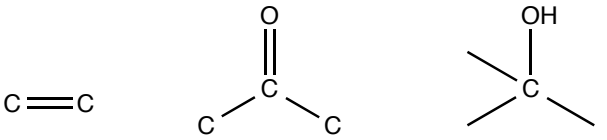

Steroid ($C_{17}$)

**Note:** All carbons are $sp^3$ hybridized

Testosterone (a steroid) - $C_{19}$

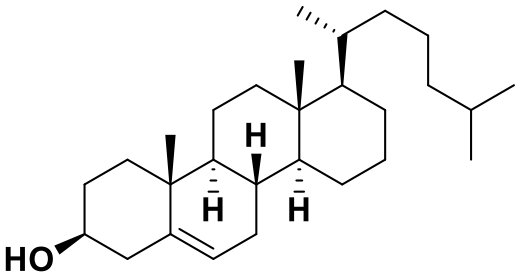
- An androgen (Male Hormone)



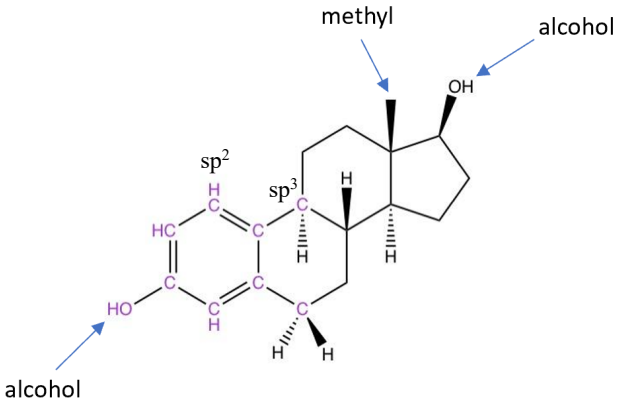

Alkene Ketone Alcohol

- Functional groups in testosterone (alkene and ketone and alcohol). Alknes are sometimes referred to as olefins.



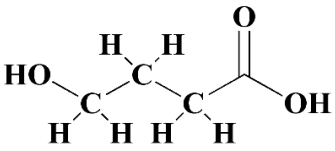

**Cholesterol**

6. **Estradiol** – (C18) estrogen steroid hormone, difference of 1 methyl group



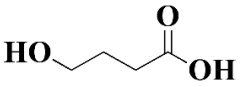

Female hormone
All purple atoms are in the same plane

7. **γ-Hydroxybutyric acid (4C)**




Open chain form

**γ -Hydroxybutyric acid**




Bond line form

MF = $C_4H_8O_3$