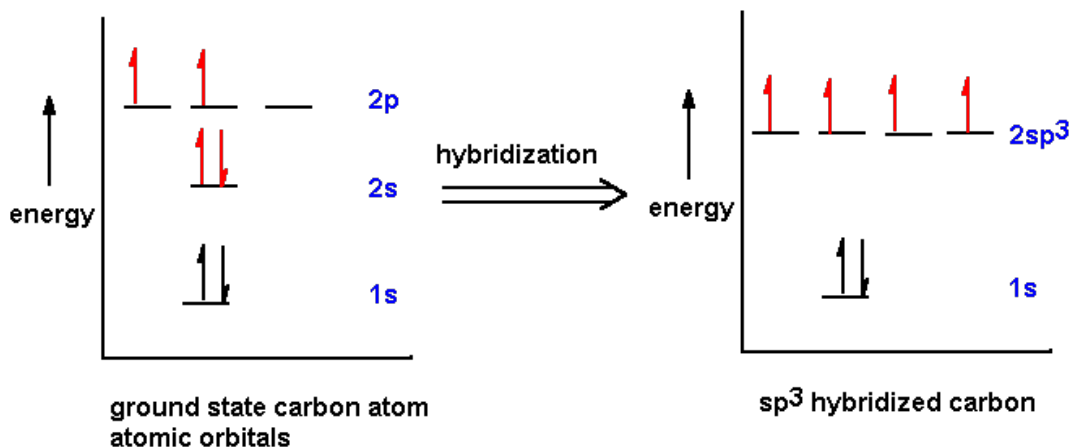


Hybridization:

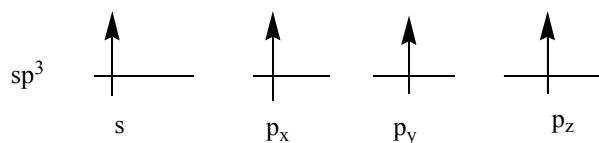
- Mixing of atomic orbitals (with the wrong geometry for bonding) to form hybrid orbitals with the correct geometry for bonding
- Will only happen for bonding

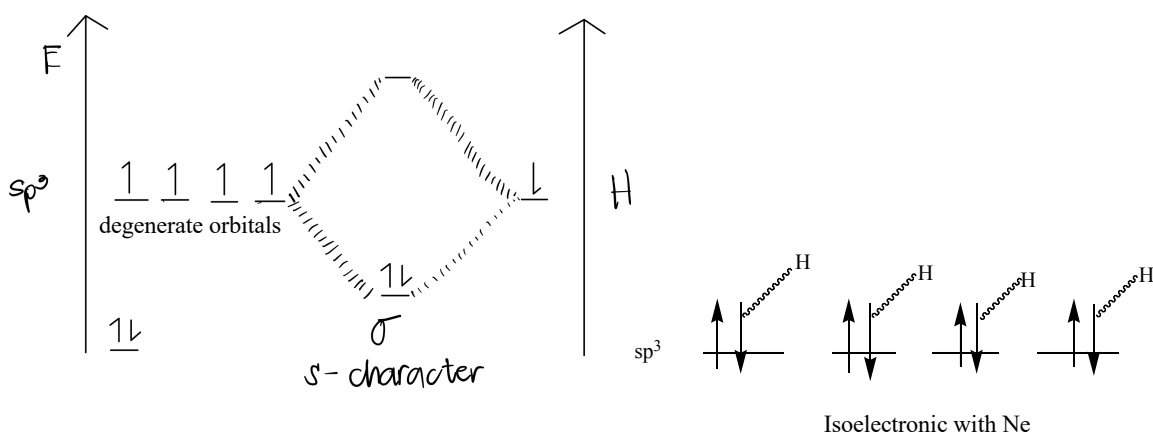
LCAO

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

**sp³ 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
- sp³ orbitals are lower in energy than 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 → sp² + s
- C = C → one is sp² + sp² and one is p + p



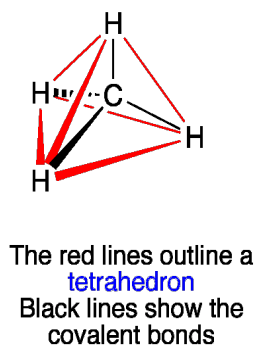
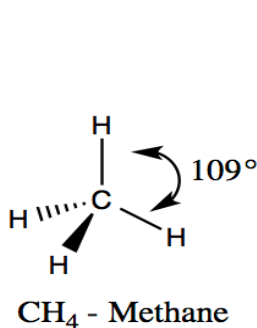


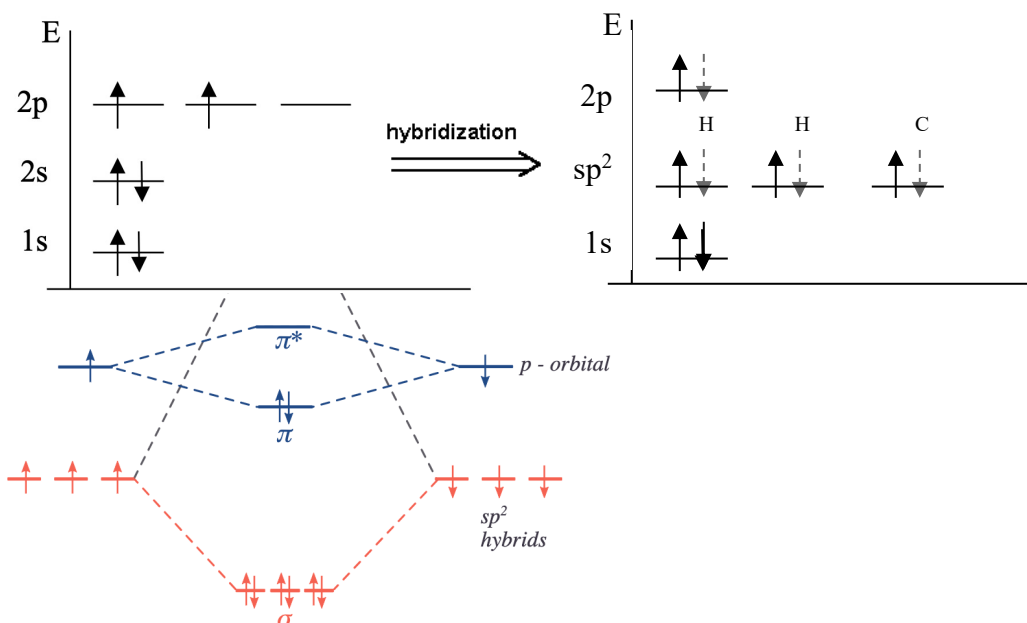
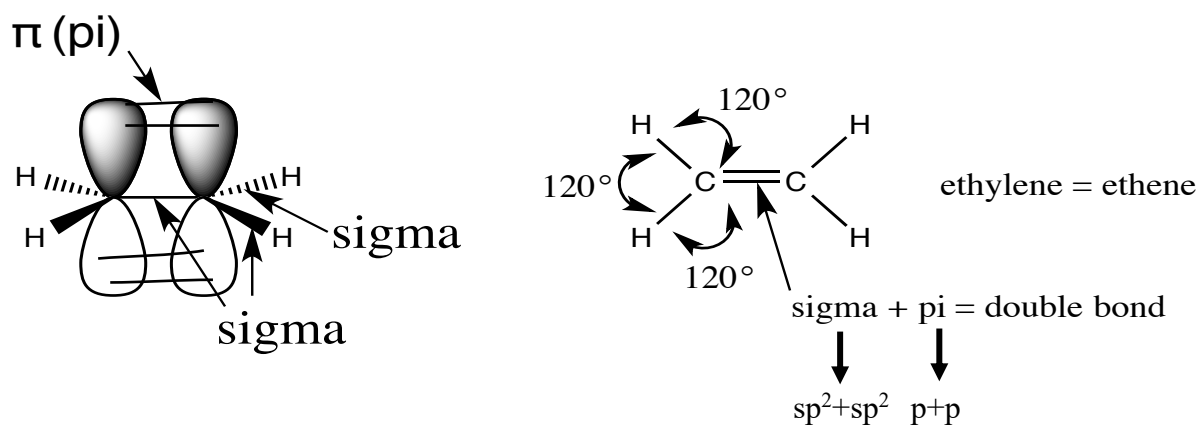
sp^2 Hybridization

- 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)

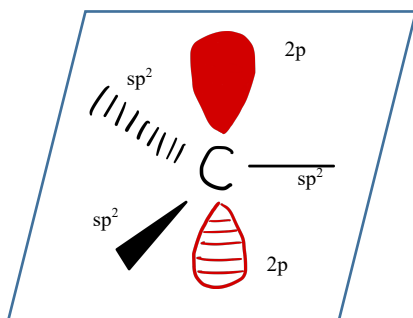
Drawing Molecules

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





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

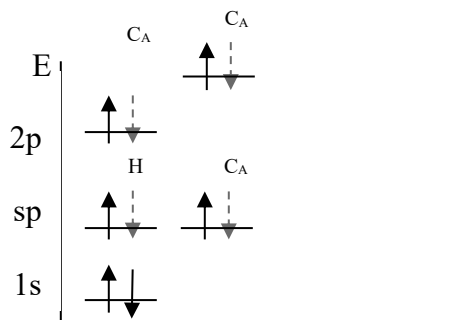
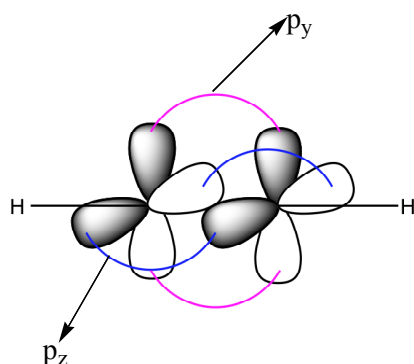
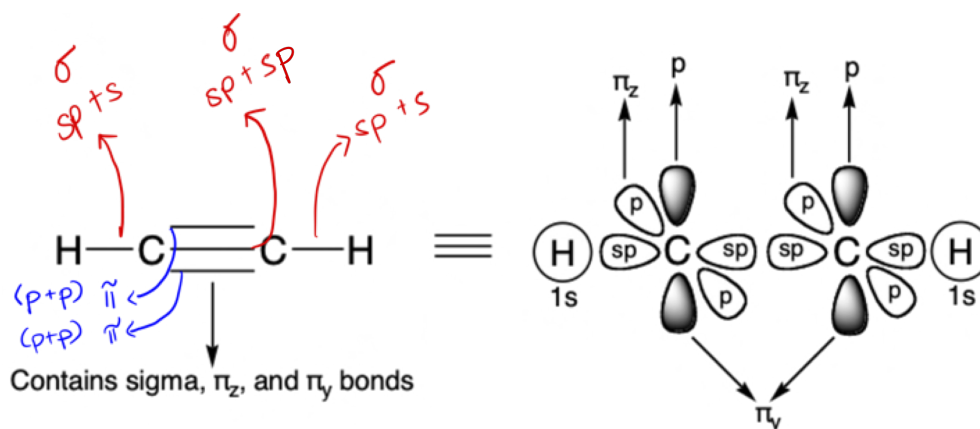


$p + p \rightarrow \pi$ molecular orbital

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

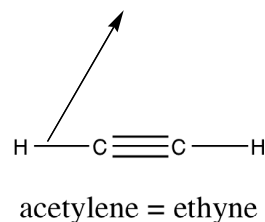
sp Hybridization

- 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:**

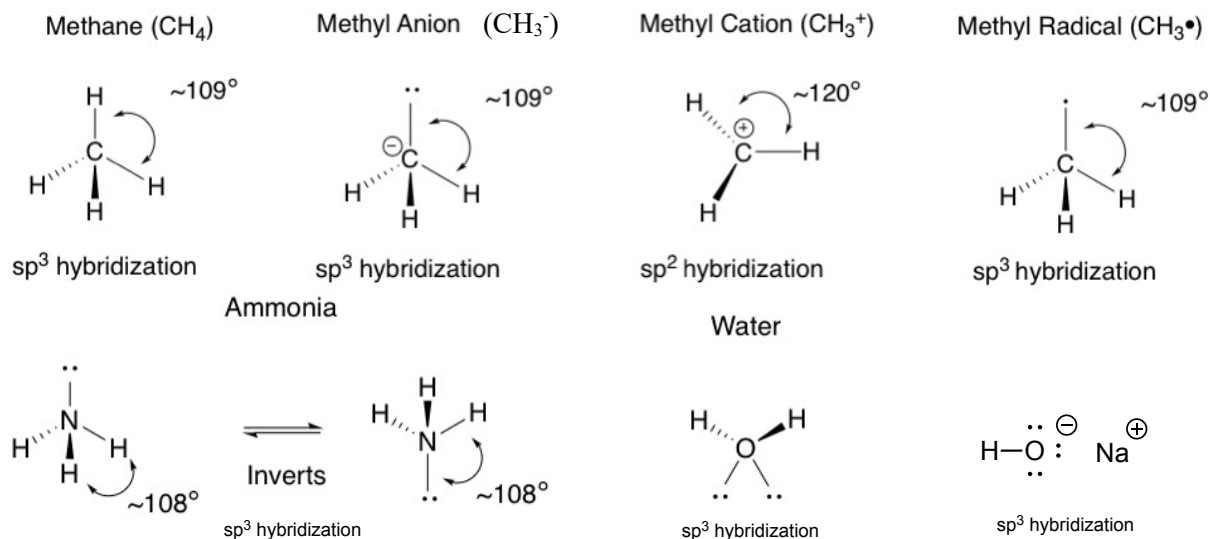
One sigma bond between the carbons plus two pi bonds formed through p_y and p_z

sigma (s of H and sp of C)

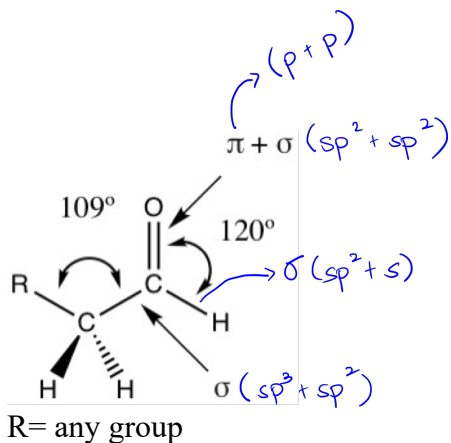


Hybridization (sp^3 vs sp^2)

- 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)

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

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



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

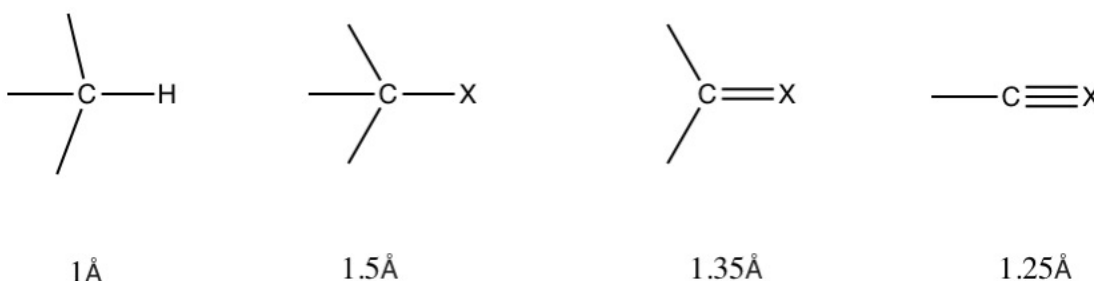
The carbonyl carbon is sp^2 hybridized, the atoms attached to it have a bond angle of 120°

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

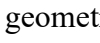
- Geometry is dictated based on filled orbitals moving as far apart as possible
- A bond length between hydrogen and a 2nd row element is approximately 1Å

NOTE THE FOLLOWING (Estimated bond length between atoms)



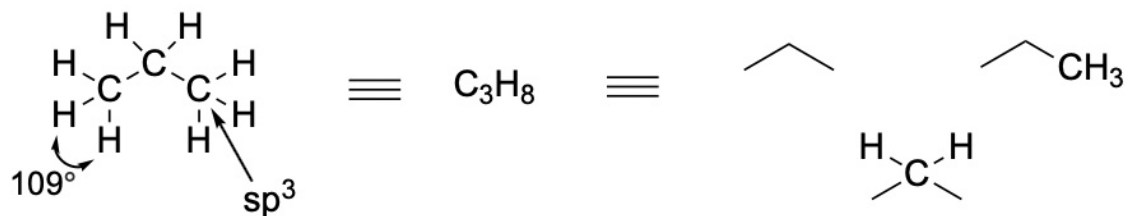
X = C, O, N

Representation of Molecules

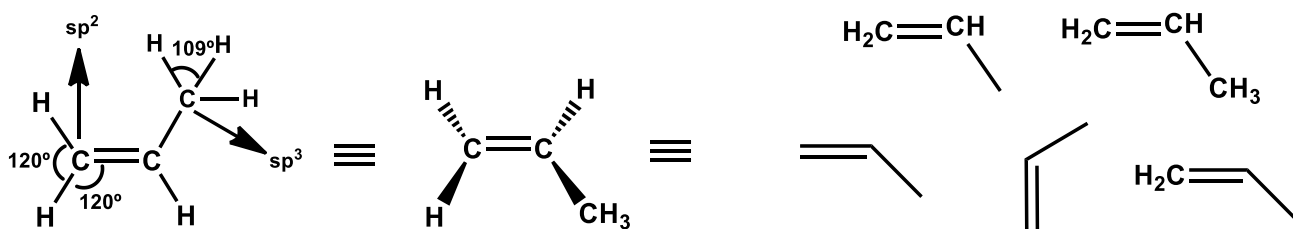
- Show only electrons in outer (valence) shell
- Line represents two bonded electrons`
- Non-bonding electrons (lone pairs) may or may not be shown
- Use element symbols, but carbon can be represented by point of angle or end of line
- Hydrogens and bonds to them from carbon are optional; show others.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

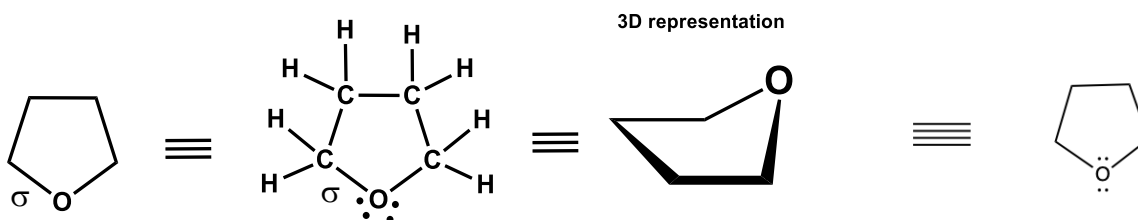
1. Propane (C₃H₈):



2. Propene (CH₃CHCH₂):



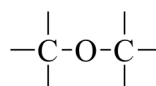
3. Tetrahydrofuran (THF)



Chemical Formula: C_4H_8O
Molecular Weight: 72.11

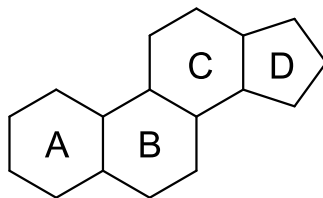
Oxygen in the stable uncharged state forms two bonds with 2 lone pairs of electrons
Nitrogen in the stable uncharged state forms three bonds with 1 lone pair of electrons

NB: Functional Group in Tetrahydrofuran is ETHER



ETHER

4. Steroid Molecule

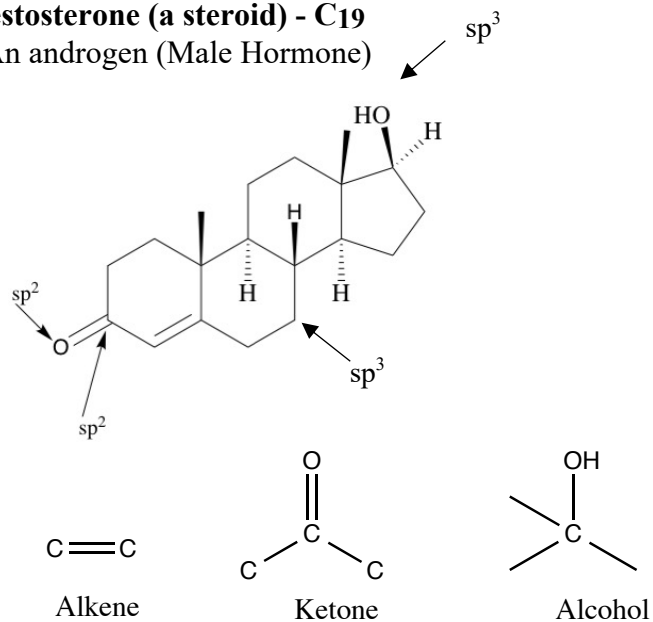


Steroid (C_{17})

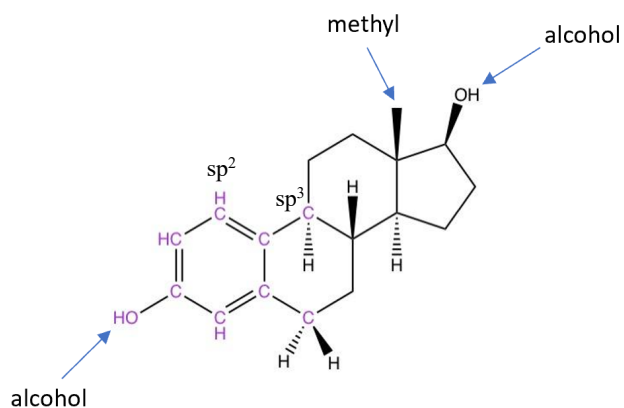
Note: All carbons are sp^3 hybridized

5. Testosterone (a steroid) - C19

- An androgen (Male Hormone)

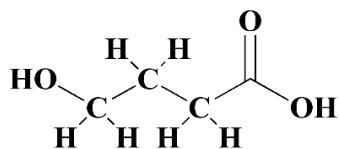


- Functional groups in testosterone (alkene and ketone and alcohol). Alknes are sometimes referred to as olefins.

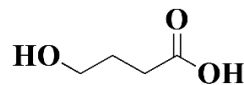
6. Estradiol – (C18) estrogen steroid hormone, difference of 1 methyl group

Female hormone

All purple atoms are in the same plane

7. γ -Hydroxybutyric acid (4C)

Open chain form

 γ -Hydroxybutyric acid

Bond line form

