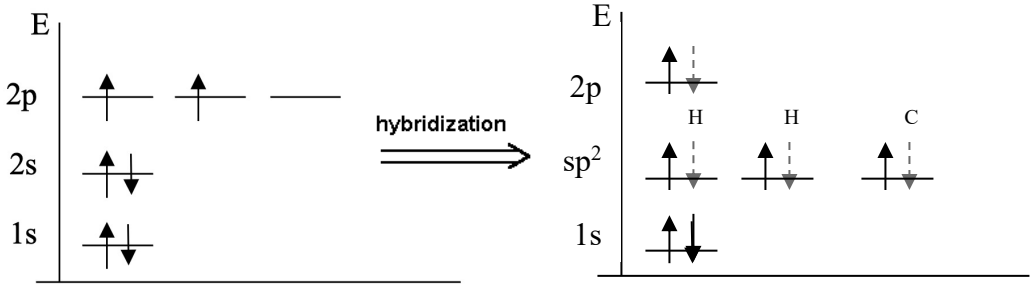
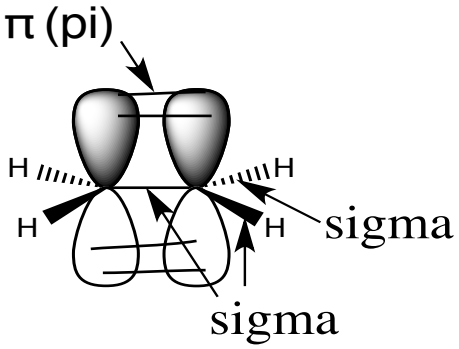
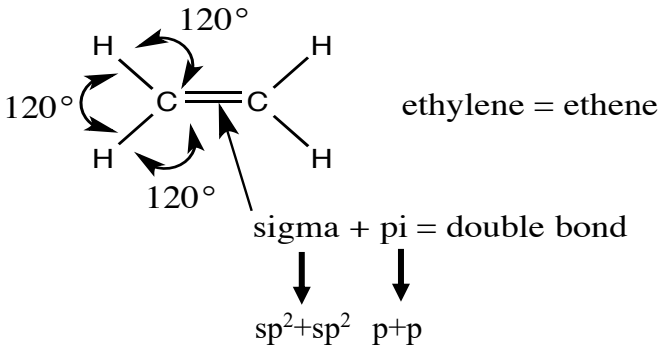
sp^2 Hybridization

- Double bonds
- Planar geometry
- Angle between two atoms: 120°
- No free rotation around double bonds
- Overlap of atomic orbitals with s component gives sigma molecular orbital (bond)
- Overlap of p atomic orbitals with s component gives pi molecular orbital (bond)



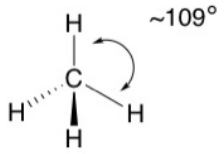




- Each line in a structure represents 2 e^-
- Solid wedge ( ): Toward you / out of the page
- Dashed wedge ( ): Away from you / into the page

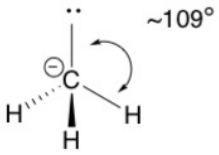
Hybridization (sp^3 vs sp^2)

Methane (CH_4)



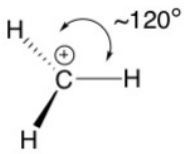
sp^3 hybridization

Methyl Anion (CH_4^-)



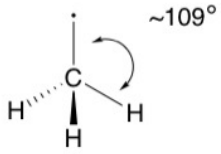
sp^3 hybridization

Methyl Cation (CH_3^+)



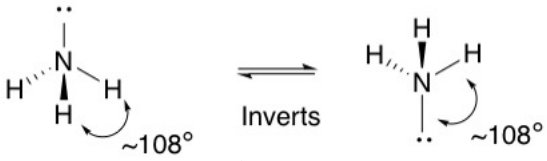
sp^2 hybridization

Methyl Radical ($CH_3\bullet$)



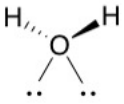
sp^3 hybridization

Ammonia

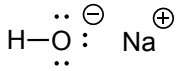


sp^3 hybridization

Water



sp^3 hybridization



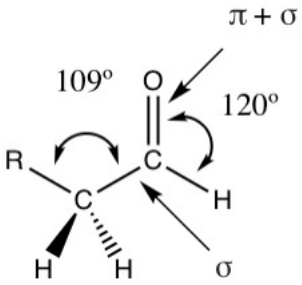
sp^3 hybridization

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

no free rotation around double bonds (overlap of p orbitals to form pi (π) bond prevents that)

e.g.

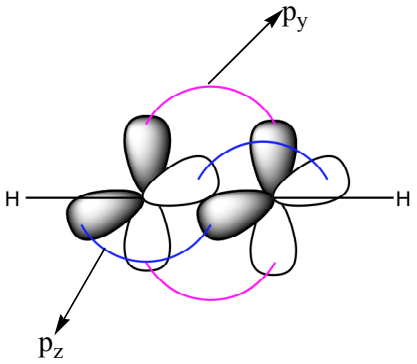
1. **Aldehyde**



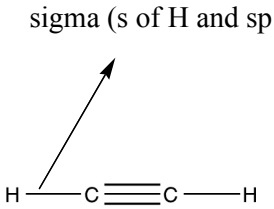
The CH_2 is sp^3 hybridized, the atoms attached to it have a bond angle of 109º
The carbonyl carbon is sp^2 hybridized, the atoms attached to it have a bond angle of 120º
The oxygen contains two lone pairs (not drawn), it is sp^2 hybridized

Hybridization: sp

- Triple bonds
- Linear geometry
- No free rotation around triple bonds



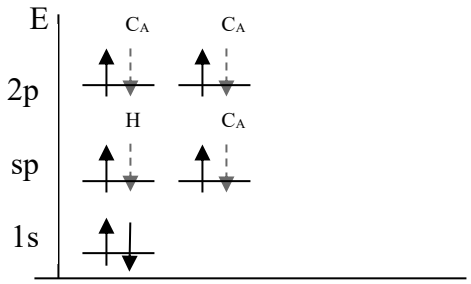
Triple bond:
One sigma bond between the carbons plus two pi bonds formed through p_y and p_z



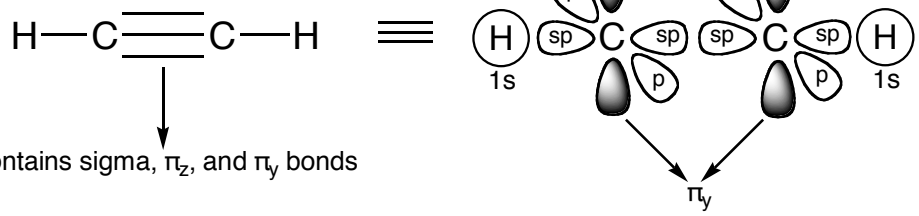
acetylene = ethyne

<u>sp Hybridization</u>

- Triple bonds
- Linear geometry
- No free rotation around triple bonds
- Angle between two atoms: 180°



e.g. Acetylene/Ethyne



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

NOTE THE FOLLOWING (Estimated bond length between atoms)

1Å = 10^{-8} cm 1.5Å 1.35Å 1.25Å

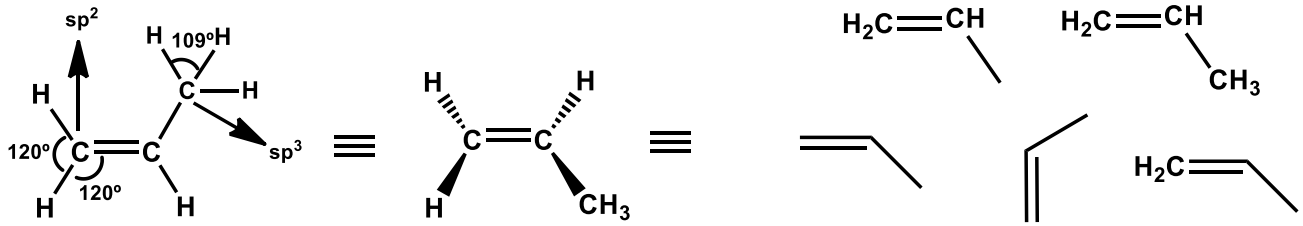
X = C, O, N

<u>Representation of Molecules</u>

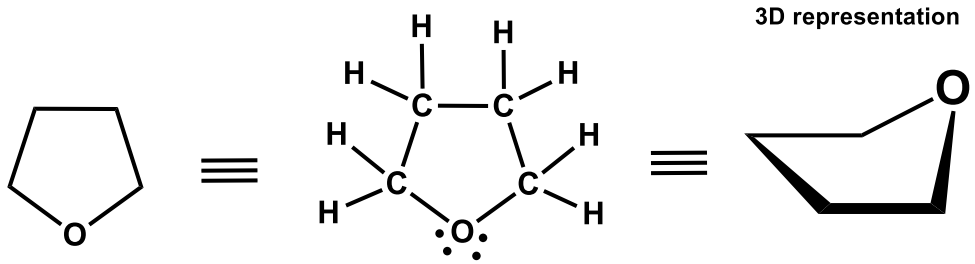
- Show only electrons in outer (valence) shell
- Non-bonding electrons (lone pairs) may or may not be shown
- Use element symbols, but carbon can be represented by point of angle or end of line
- Hydrogens and bonds to them from carbon are optional; show others.
- Each line in a structure represents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

Examples:

Propene:



1. Tetrahydrofuran (THF)

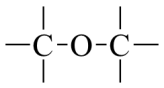


Chemical Formula: C_4H_8O
Molecular Weight: 72.11

NB: Oxygen in the stable uncharged state forms two bonds with 2 lone pairs of electrons

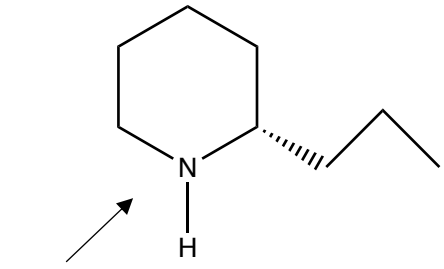
NB: Nitrogen in the stable uncharged state forms three bonds with 1 lone pair of electrons

NB: Functional Group in Tetrahydrofuran is ETHER

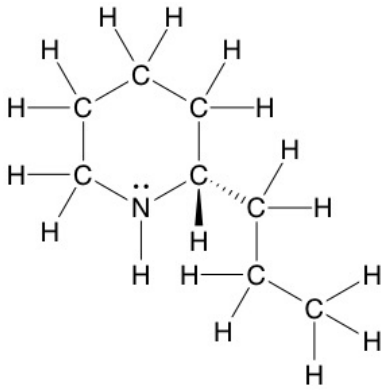


ETHER

2. Conine (Poison Hemlock)

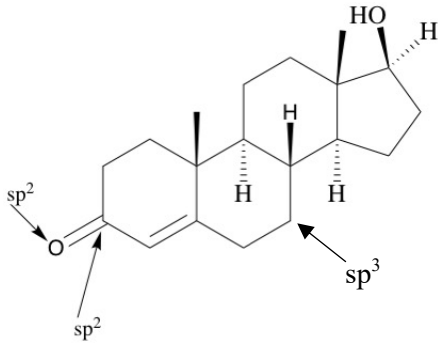


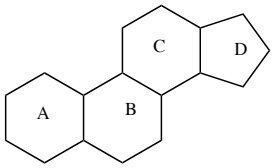
Amine



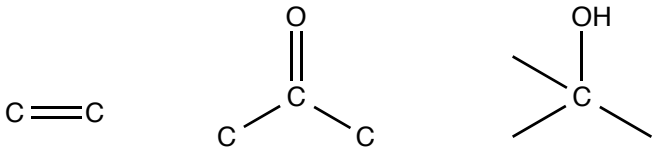
Chemical Formula: $C_8H_{17}N$
Molecular Weight: 127.23

3. Testosterone (a steroid) - C_{19}





A Steroid, Ring Nomenclature A, B, C, D etc

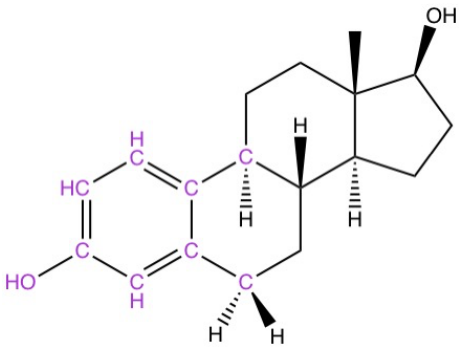


Alkene Ketone Alcohol

CH_3 = Methyl
CH_2 = Methylene
CH = Methine

Functional groups in testosterone (alkene and ketone and alcohol)

4. Estradiol - C_{18}



Female hormone
All purple atoms are in the same plane

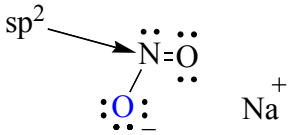
Formal Charge

- Convention to keep track of charges
- ∑ (sum of) of formal charges on all atoms in a molecule = overall charge on molecule

Rules for calculating formal charge

- 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

1. Sodium Nitrite –$NaNO_2$



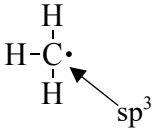
Formal Charge on Nitrogen

+7 (number of protons)
-2 (1s electrons)
-2 (unshared electrons)
½ x 6 = -3 (1/2 of shared electrons)
0

Single bonded oxygen (O)

+8 (number of protons)
-2 (1s electrons)
-6 (unshared electrons)
½ x 2 = -1 (1/2 of shared electrons)
-1

2. Methyl Radical

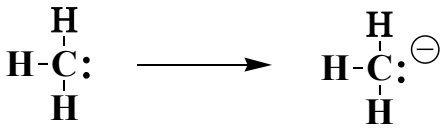


Formal Charge on Carbon

+6 (number of protons)
-2 (1s electrons)
-1 (unshared electrons)
½ x 6 = -3 (1/2 of shared electrons)
0

H· = hydrogen atom (radical)

3. Methyl anion

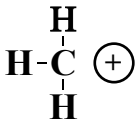


Formal Charge on Carbon
+6 (number of protons)
-2 (1s electrons)
-2 (unshared electrons)
½ x 6 = -3 (1/2 of shared electrons)
-1

Overall charge on the methyl anion is = **-1**

4. Methyl cation

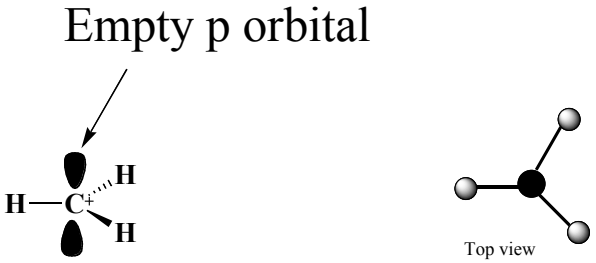
- (sp^2 hybridized carbon, planer shape**)**
- can be reactive intermediate in principle



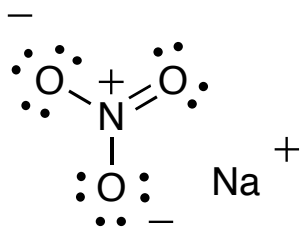
Formal Charge on Carbon
+6 (number of protons)
-2 (1s electrons)
0 (unshared electrons)
½ x 6 = -3 (1/2 of shared electrons)
+1

Overall charge on the methyl anion is = **+1**

$H:^{\ominus}$ = hydride anion



5. Sodium Nitrate – $NaNO_3$



Formal Charge on Nitrogen:
+7 (number of protons)
-2 (1s electrons)
0 (unshared electrons)
½ x 8 = -4 (1/2 of shared electrons)
+1

Double bonded oxygen:
+8 (number of protons)
-2 (1s electrons)
-4 (unshared electrons)
½ x 4 = -2 (1/2 of shared electrons)
0

Single bonded oxygen (both):
+8 (number of protons)
-2 (1s electrons)
-6 (unshared electrons)
½ x 2 = -1 (1/2 of shared electrons)
-1

Overall charge on the nitrate anion is = +1 + 0 – 1 – 1 = **-1**