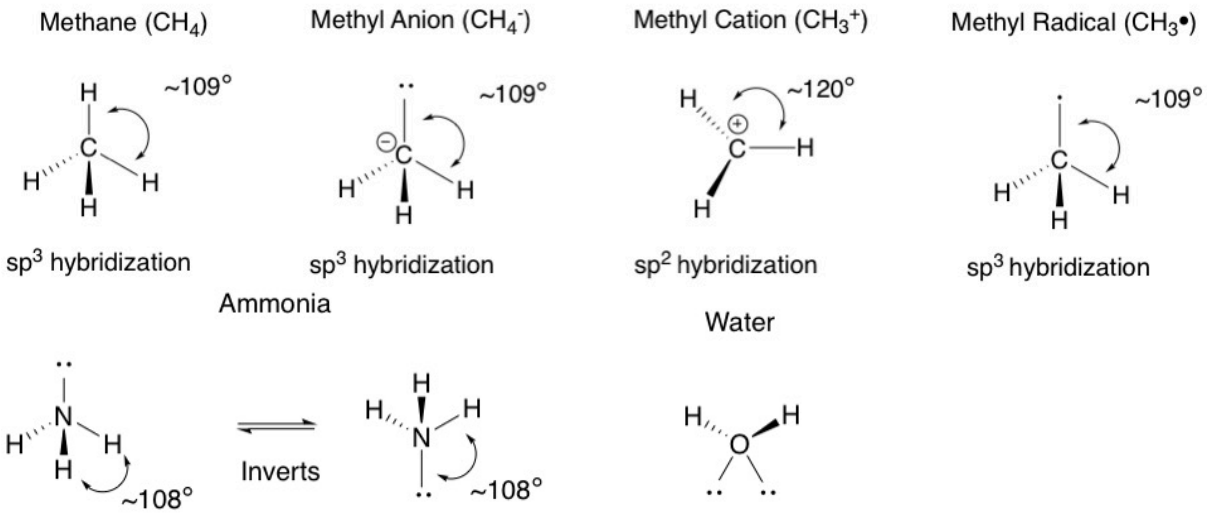
Chem 261 Sep 11, 2018

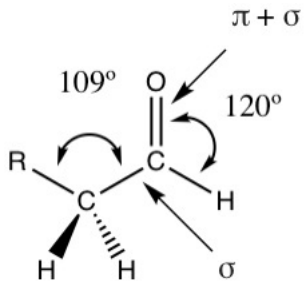
Hybridization (sp^3 vs sp^2)



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.

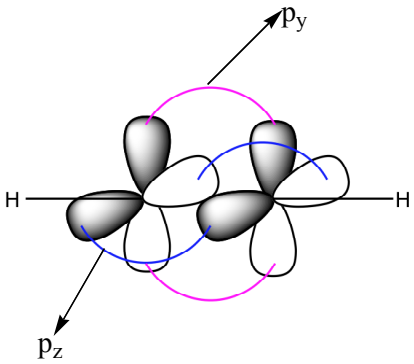
1. **Aldehyde**



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

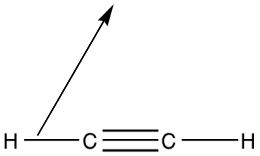
Hybridization: sp

- 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

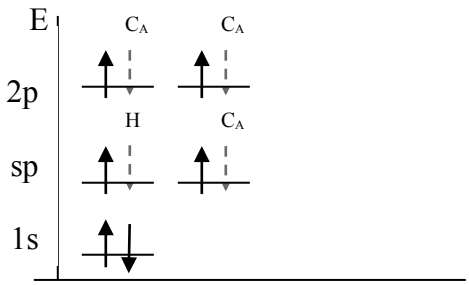
sigma (s of H and sp of C)



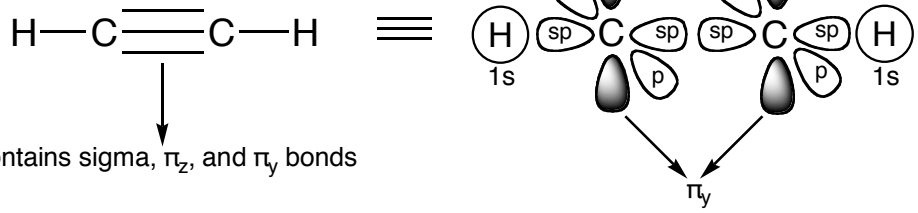
acetylene = ethyne

sp Hybridization

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

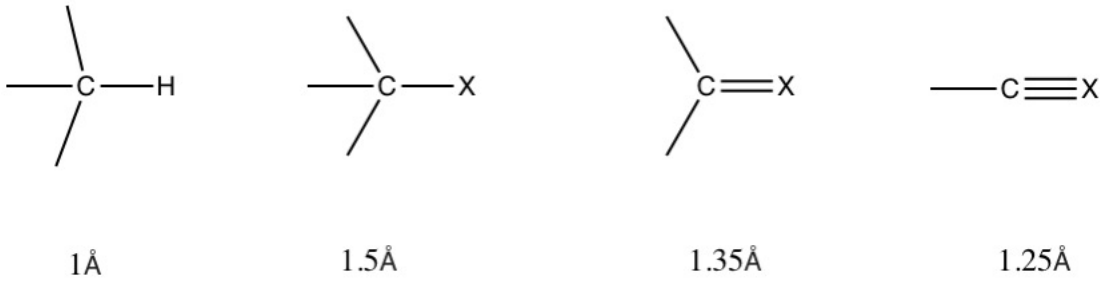


e.g. Acetylene/Ethyne



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

NOTE THE FOLLOWING (Estimated bond length between atoms)



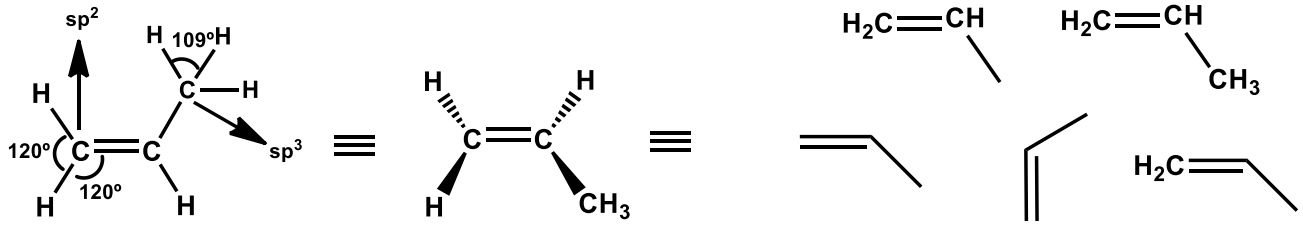
X = C, O, N, F

<u>Representation of Molecules</u>

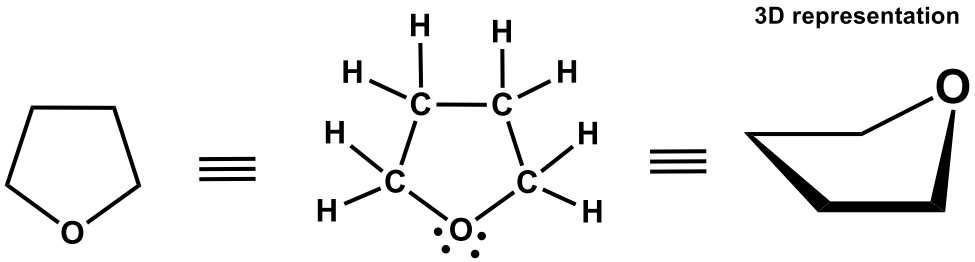
- Show only electrons in outer (valence) shell
- Non-bonding electrons (lone pairs) may or may not be shown
- Use element symbols, but carbon can be represented by point of angle or end of line
- Hydrogens and bonds to them from carbon are optional; show others.
- Each line in a structure represents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

Examples:

Propene:



1. Tetrahydrofuran (THF)

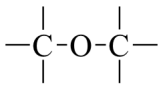


Chemical Formula: C_4H_8O
Molecular Weight: 72,11

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

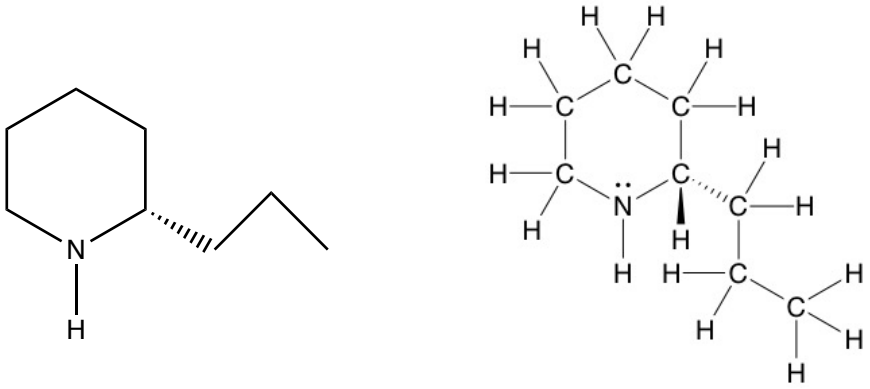
NB: Nitrogen in the stable uncharged state forms three bonds with 1 lone pair of electrons

NB: Functional Group in Tetrahydrofuran is ETHER



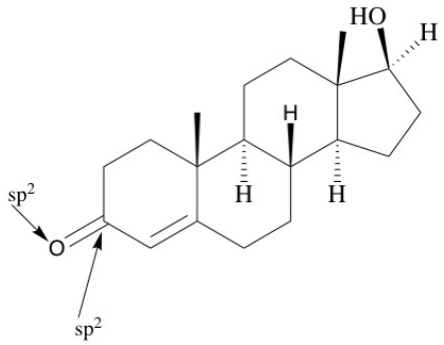
ETHER

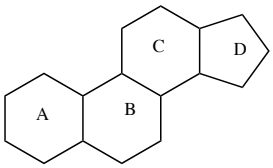
2. Conine (Poison Hemlock)



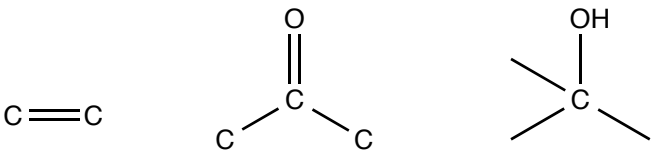
Chemical Formula: $C_8H_{17}N$
Molecular Weight: 127.23

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





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

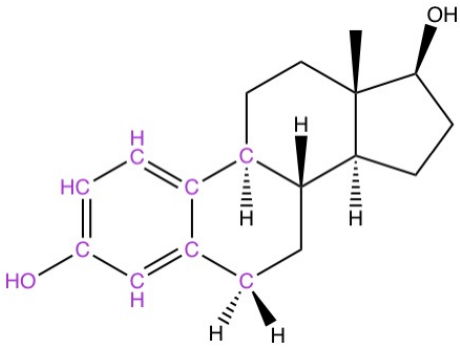


Alkene Ketone Alcohol

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

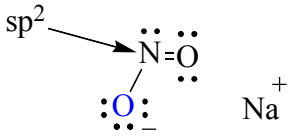
Formal Charge

- 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 –$NaNO_2$**



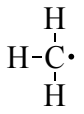
Formal Charge on Nitrogen

+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

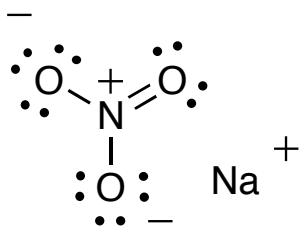
2. **Methyl Radical**



Formal Charge on Carbon

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

3. 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**