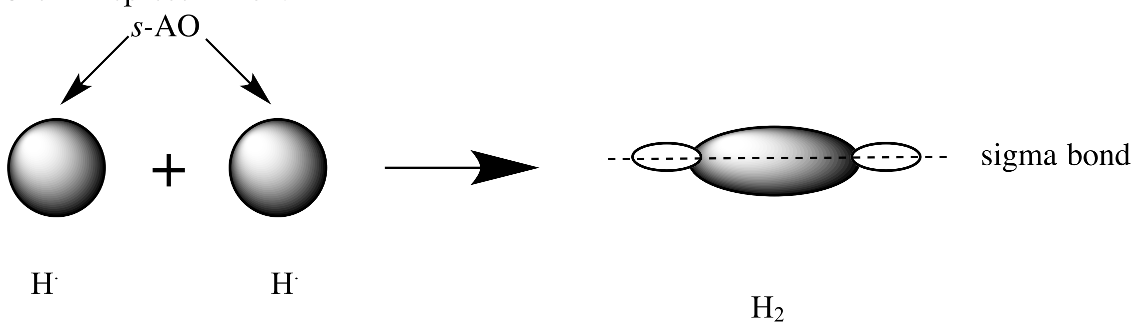
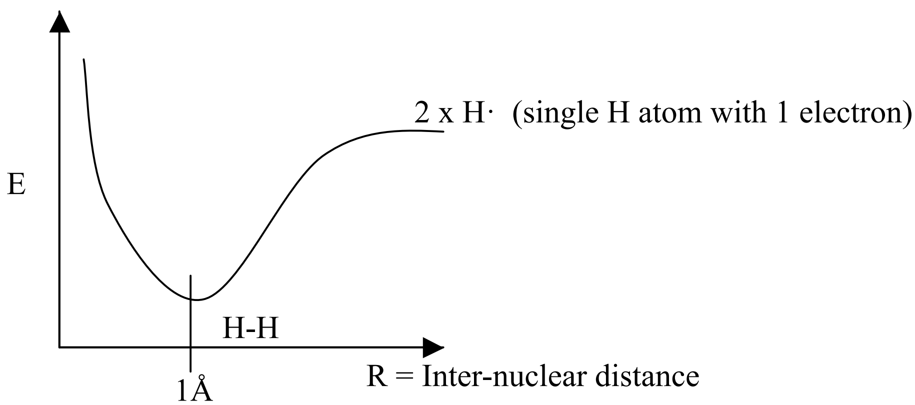
As two hydrogen atoms come together, molecular hydrogen (H_2) is formed

$$H^{\cdot} \longrightarrow H{:}H \longleftarrow {}^{\cdot}H$$

Orbital representation:



Energy diagram of two hydrogen atoms interacting to form a bond:

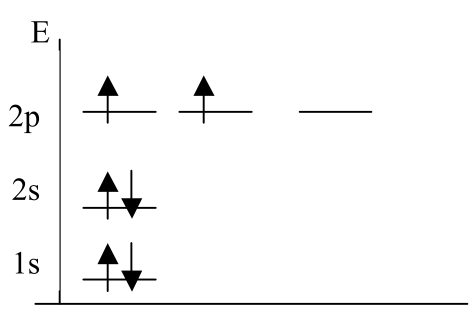


1Å is the average H-H bond distance

Electronic configuration of carbon (C):

- Atomic number = 6
- Atomic weight = 12

Carbon (C)



- Carbon needs to gain or lose $4e^-$ to get an inert gas configuration, but this would result in unfavourable charge buildup:

- C^{4+} is isoelectronic with He

- C^{4-} is isoelectronic with Ne

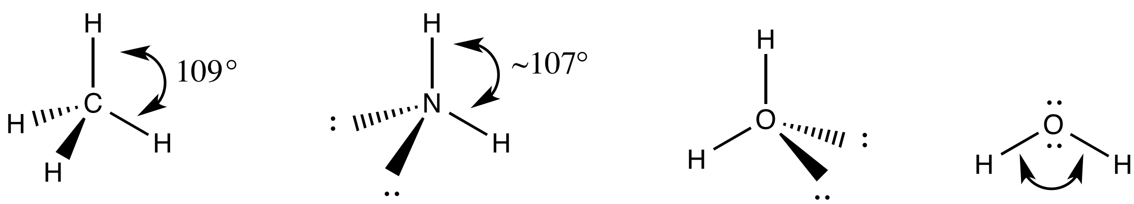
- So, carbon makes up to 4 bonds to share $4e^-$ (covalent bonding)

Hybridization:

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

sp^3 Hybridization

- Single bonds
- Tetrahedral geometry
- Angle between two H atoms in methane: 109°, close to that with other elements
- Often free rotation around single bonds
- Overlap of atomic orbitals with s component gives sigma molecular orbital (bond)



CH_4 - Methane NH_3 - Ammonia H_2O - Water

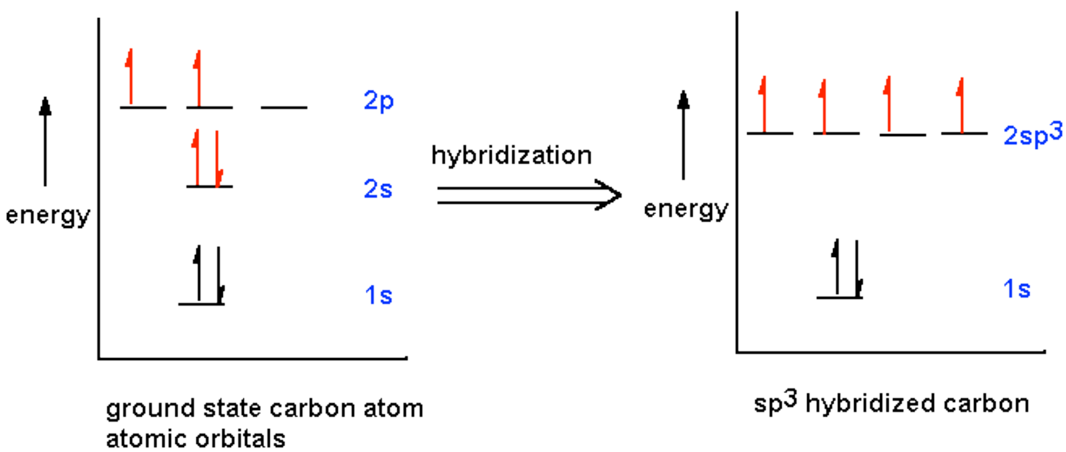
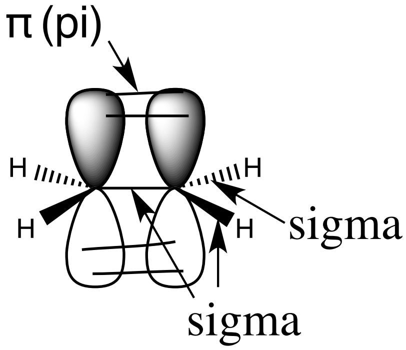
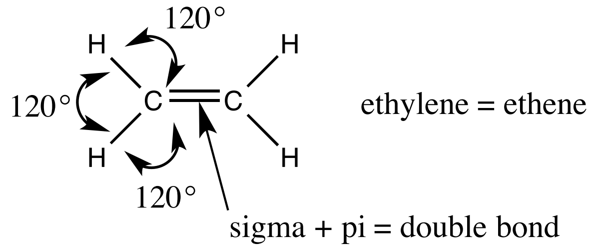


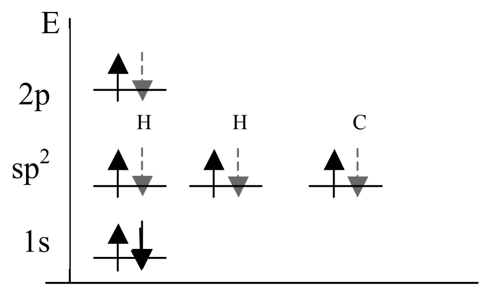
Figure: Hybridization of 2nd shell *s* (one) orbitals and *p* (three) orbitals of carbon

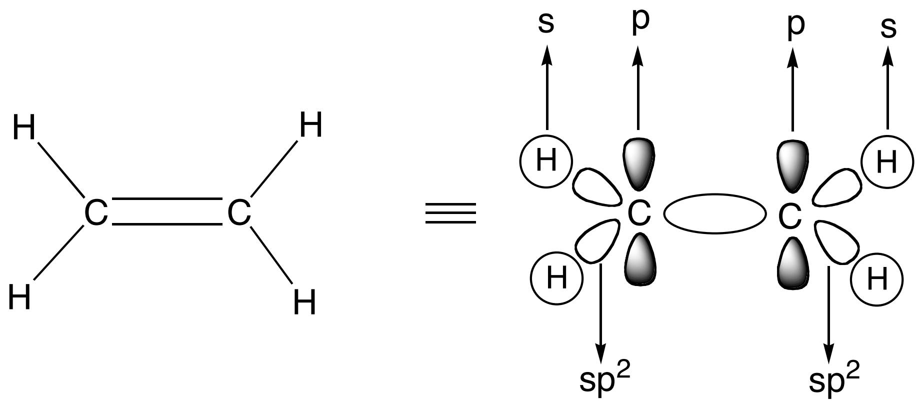
sp^2 Hybridization

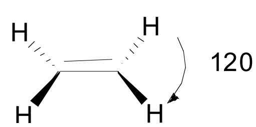
- Double bonds
- Planar geometry
- Angle between two atoms: 120°
- No free rotation around double bonds
- Overlap of atomic orbitals with s component gives sigma molecular orbital (bond)
- Overlap of p atomic orbitals with s component gives pi molecular orbital (bond)







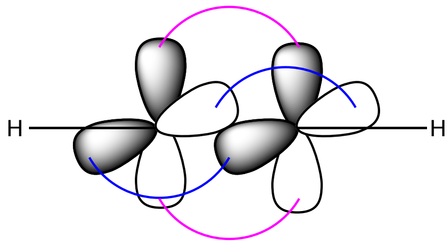




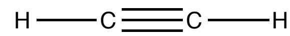
- When atomic orbitals overlap they form molecular orbitals.
- Double bond contains one σ bond and one π bond.
- σ bond has free rotation.
- π bond fixes geometry, does not allow for around the double bond.

sp Hybridization

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



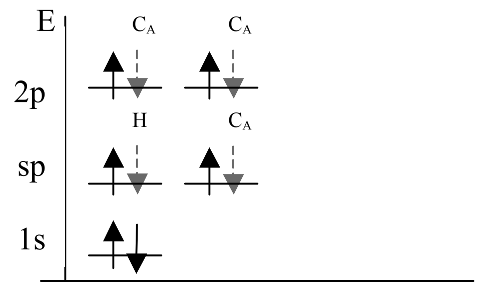
Triple bond:
One sigma bond between the carbons plus two pi bonds formed through p_y and p_z



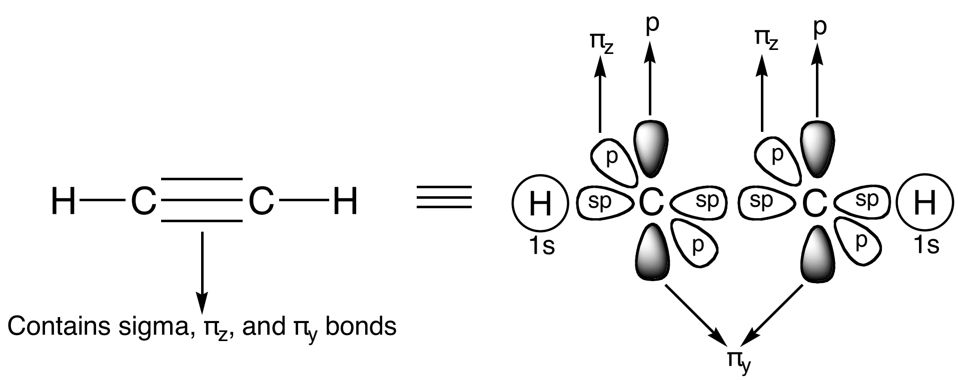
acetylene = ethyne

<u>sp Hybridization</u>

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



e.g.) Acetylene/Ethyne



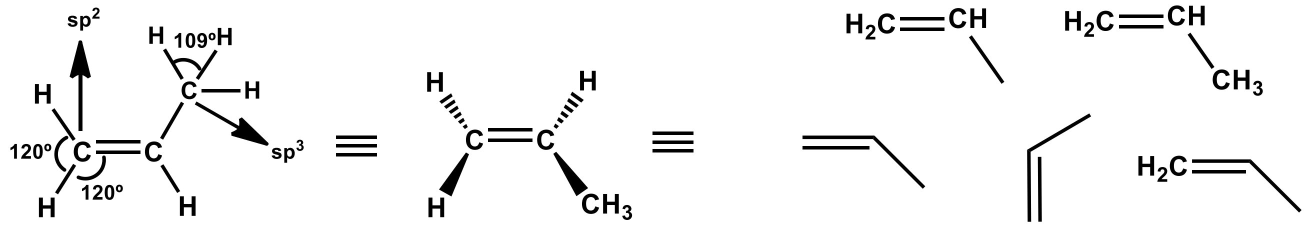
<u>Representation of Molecules</u>

- Show only electrons in outer (valence) shell
- Non-bonding electrons 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

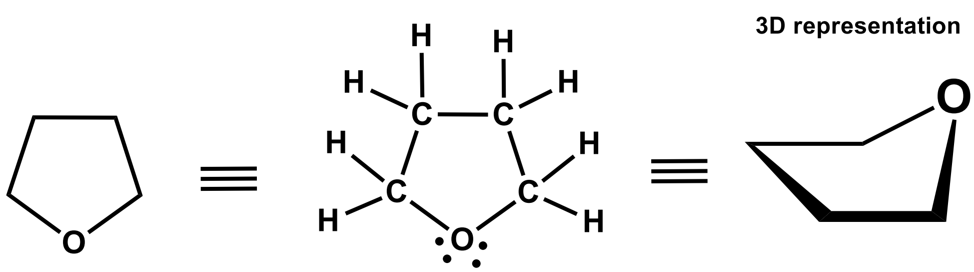
-

Examples:

1. C_3H_3 propene

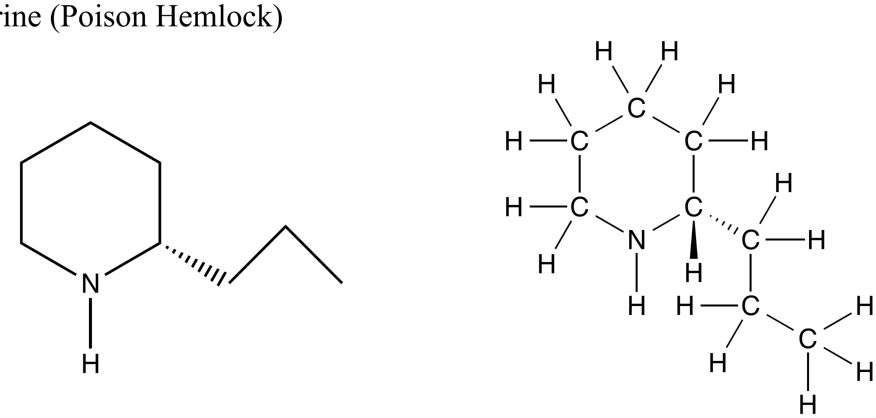


2. Tetrahydrofuran (THF)



Chemical Formula: C_4H_8O
Molecular Weight: 72,11

3. Corine (Poison Hemlock)



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

CH_3 Methyl
CH_2 Methylene
CH Methine

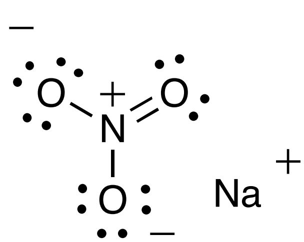
Formal Charge

- 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 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

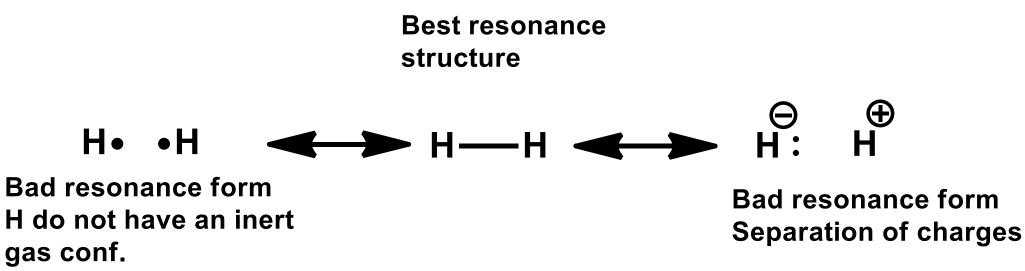
Overall charge on the nitrate anion is = +1 + 0 – 1 – 1 = **-1**

Resonance Structures: Different drawings of the same molecule.

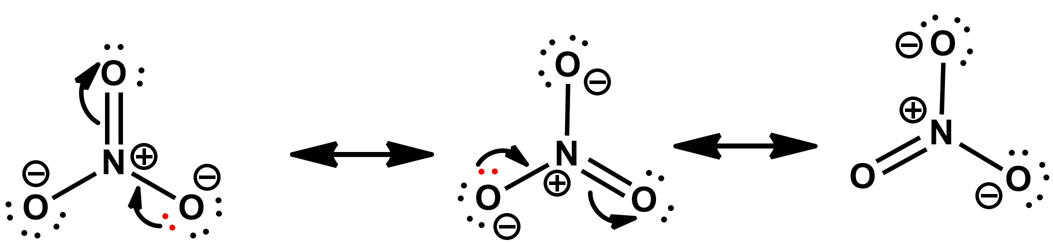
- Move the electrons, keeping the position of the atoms same
- Maintain inert gas configuration around each atom
- Avoid separation of charges
- Avoid like-charges on adjacent atoms
- Double headed arrow (⟷) is used indicate resonance forms

Examples

1. **Hydrogen gas, H_2**



2. **Nitrate anion (NO_3^-)**



The structures above are all equally valid; only one needs to be drawn.

Arrow pushing convention: Book keeping of electrons

Movement of an electron pair

Movement of a single electron