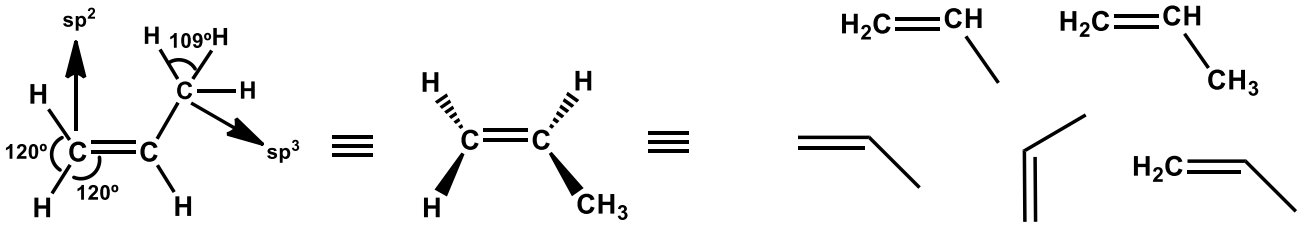
Representation of Molecules

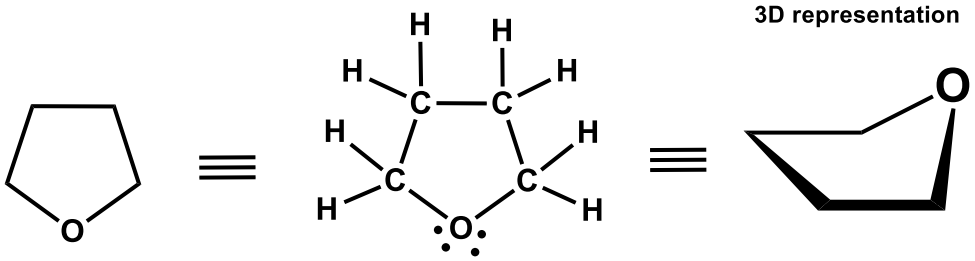
- Show only electrons in outer (valence) shell
- Non-bonding electrons may not be shown
- Use element symbols, but carbon can be represented by point of angle or end of line
- Hydrogens and bonds to them from carbon are optional, show others

Examples:

1. C_3H_3 propene

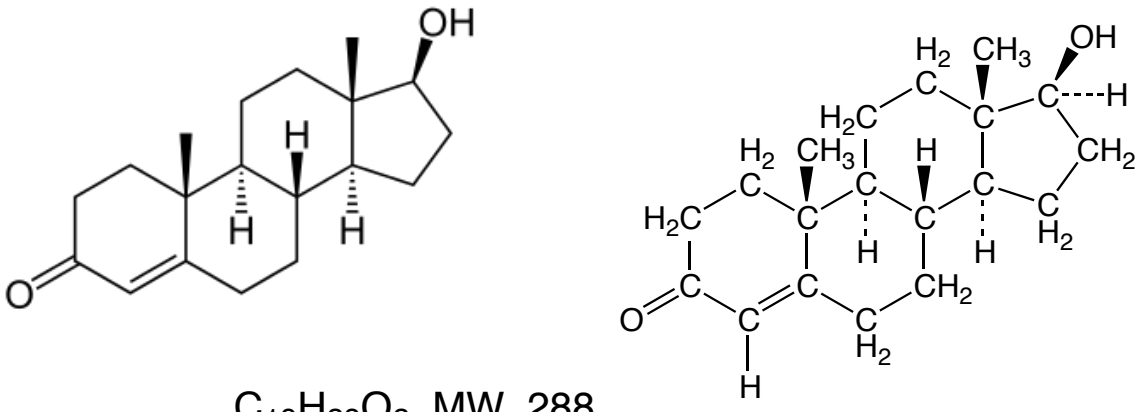


2. Tetrahydrofuran (THF)



Chemical Formula: C_4H_8O
Molecular Weight: 72,11

3. Testosterone: Principal male sex hormone



$C_{19}H_{28}O_2$ MW 288

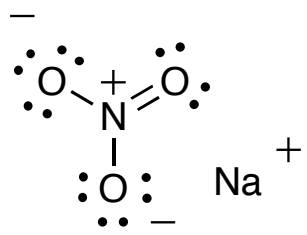
Formal Charge

- 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:

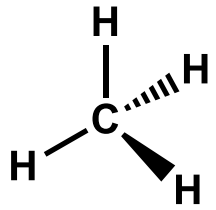
+8 (number of protons)
-2 (1s electrons)
-4 (unshared electrons)
½ x 4 = -2 (1/2 of shared electrons)
0

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**

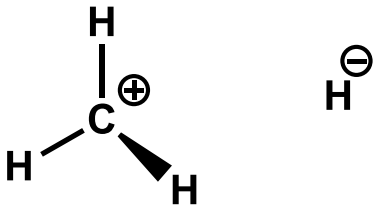
2. Methane:



Formal Charge on Carbon:
+6 (number of proton)
-2 (1s electron)
0 (unshared electrons)
½ x 8 = -4 (1/2 of shared electrons)
0

Formal Charge on Hydrogen:
+1 (number of proton)
0 (inner shell electron)
0 (unshared electrons)
½ x 2 = -1 (1/2 of shared electrons)
0

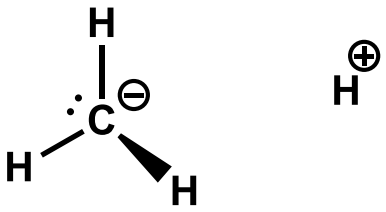
3) Methyl Cation:



Formal Charge on Carbon
+6 (number of protons)
-2 (inner shell e-)
-3 (1/2 shared e-)
_____
+1

Formal Charge on H^-:
+1 (number of protons)
0 (inner shell electron)
-2 (unshared electrons)
½ x 0 = 0 (1/2 of shared e-
_____
-1

4) Methyl Anion/Carbanion:



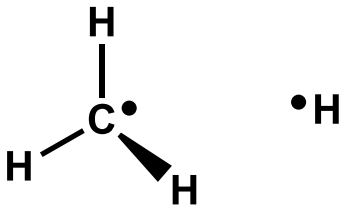
Formal Charge on Carbon:
+6 (number of proton)
-2 (1s electron)
-2 (unshared electrons)
½ x 6 = -3 (1/2 of shared electrons)
-1

Formal Charge on H^+:
+1 (number of proton)
0 (inner shell electron)
0 (unshared electrons)
½ x 0 = 0 (1/2 of shared electrons)
+1

Formal Charge on Bonded Hydrogen:

+1 (number of proton)
0 (inner shell electron)
0 (unshared electrons)
½ x 2 = -1 (1/2 of shared electrons)
0

4) Methyl Radical:



Formal Charge on Carbon:

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

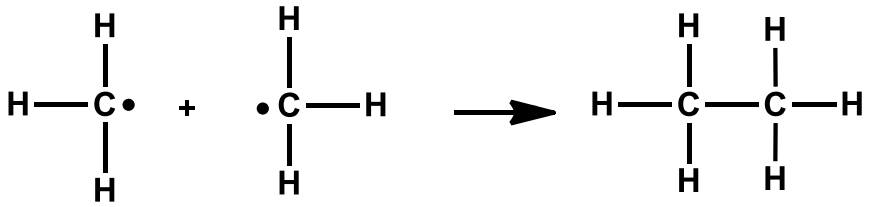
Formal Charge on Hydrogen:

+1 (number of proton)
0 (inner shell electron)
0 (unshared electrons)
½ x 2 = -1 (1/2 of shared electrons)
0

Formal Charge on $H^{\cdot}$:

+1 (number of proton)
0 (inner shell electron)
-1 (unshared electrons)
½ x 0 = 0 (1/2 of shared electrons)
0

Radicals are very reactive species because they do not have an inert gas configuration. A methyl cation will rapidly react with another methyl cation to form ethane:

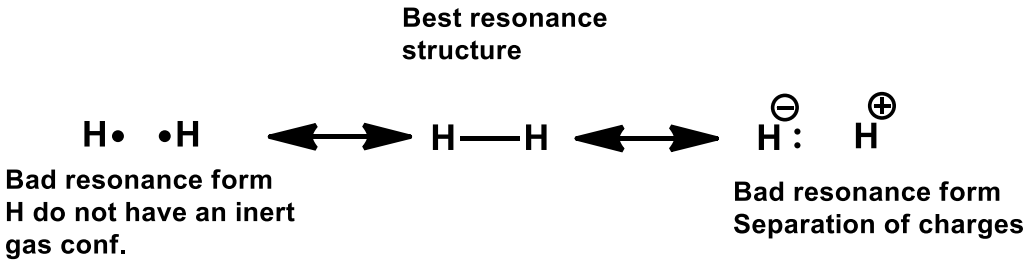


Resonance Structures: Different drawings of the same molecule.

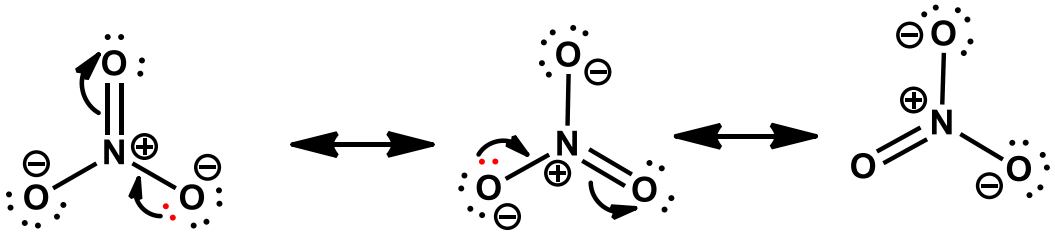
- Move the electrons, keeping the position of the atoms same
- Maintain inert gas configuration around each atom
- Avoid separation of charges
- Avoid like-charges on adjacent atoms
- Double headed arrow (⟷) is used indicate resonance forms

Examples

1. **Hydrogen gas, H_2**

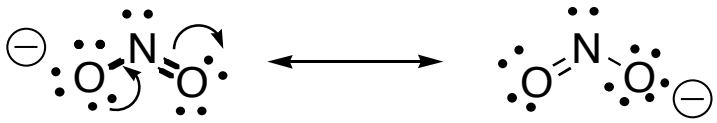


2. **Nitrate anion (NO_3^-)**



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

3. **Nitrite anion (NO_2^-)**



The two resonance structures shown above are equally valid.

Arrow pushing convention: Book keeping of electrons

Movement of an electron pair

Movement of a single electron