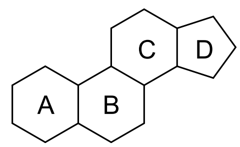
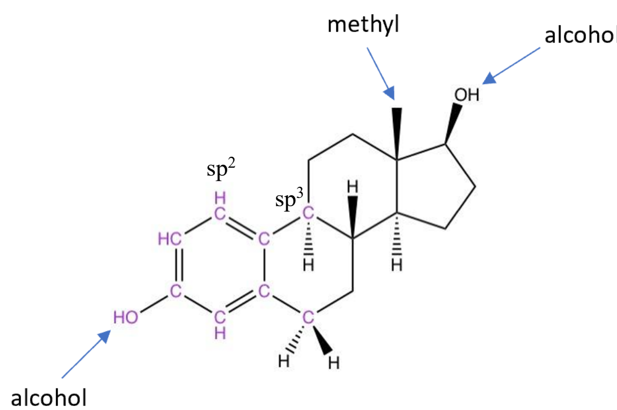
AS A REMINDER:

More examples for representation of molecules



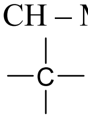
Steroid (C_{17})

1. **Estradiol** - estrogen steroid hormone
   - Discovered and elucidated by Adolf Butenant and Edward Doisy (1929)
   - 4 ton of hog ovaries → 4 mg of estradiol
   -



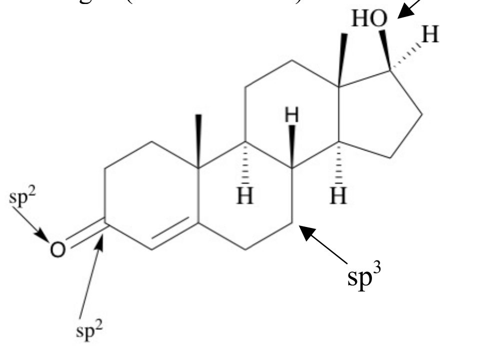
Female hormone
All purple atoms are in the same plane

Types of C:
CH_3 – Methyl
CH_2 – Methylene
CH – Methine

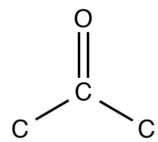


- Quaternary carbon

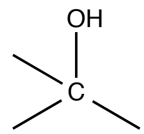
2. **Testosterone (a steroid) - C19**
   - An androgen (Male Hormone)



Alkene



Ketone

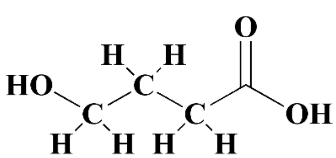


Alcohol

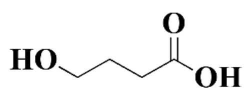
Functional groups in testosterone (alkene and ketone and alcohol)

DRAWING CHEMICAL STRUCTURES

γ -Hydroxybutyric acid



Open chain form

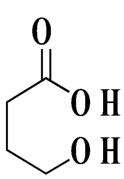


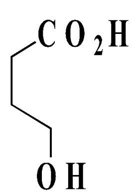
Bond line form

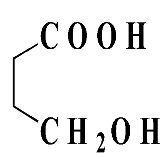
MF = $C_4H_8O_3$

- **C=O** is a carbonyl
- **COOH** is a carboxylic acid

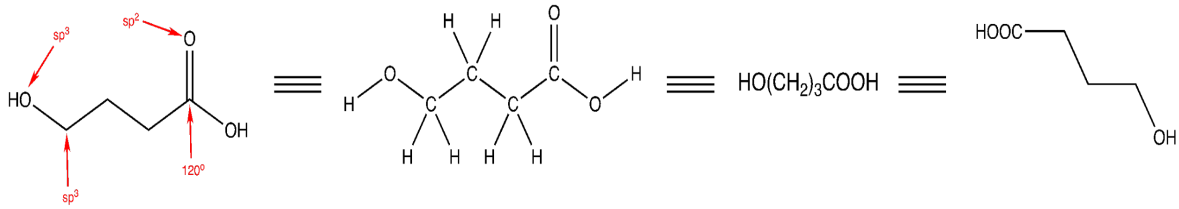
The above compound can also be represented in the following forms, resulting from the free rotation of single bonds (sigma).







Example:



Note: Single bonds, in general, have free rotation

Formal Charge

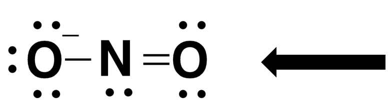
- Convention to keep track of charges
- ∑ (sum of) of formal charges on all atoms in a molecule = overall charge on molecule

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

Examples:

1. **$NaNO_2$ (sodium nitrite;** food preservative**)**
   Nitrite anion



Formal charge

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

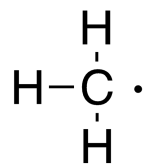
Single bonded oxygen:

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

Central N:

+7 (number of protons)
-2 (1s e^-)
-2 (unshared e^-)
-3 (1/2 shared e^-)
= **0**

2. **Methyl radical (sp^3, tetrahedral)**



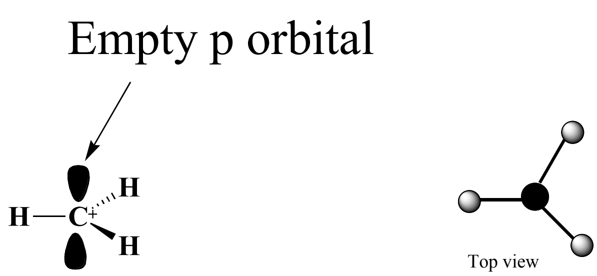
Formal Charge on Carbon
+6 (number of protons)
-2 (1s electrons)
1 (unshared electrons)
½ x 6 = -3 (1/2 of shared electrons)
0

Overall charge on the methyl anion is = **0**
Very unstable since it doesn't have an inert gas configuration

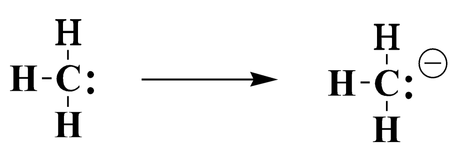
3. **Methyl cation (carbocation, sp^2, planar)**
   - (sp^2 hybridized carbon, planar shape)
   - can be reactive intermediate in principle

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**



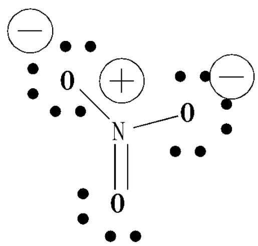
4. **Methyl anion (sp^3, tetrahedral)**



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**

5. Sodium Nitrate ($NaNO_3$)

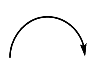


Formal Charge on Nitrogen

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

Resonance Structures: Different drawings (or pictures) of the same molecule made by moving electrons but not atoms

- Move the electrons, keeping the position of the atoms same
- Good resonance structures:
  - 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 Fish Hook and double headed arrows are used to show electron movement

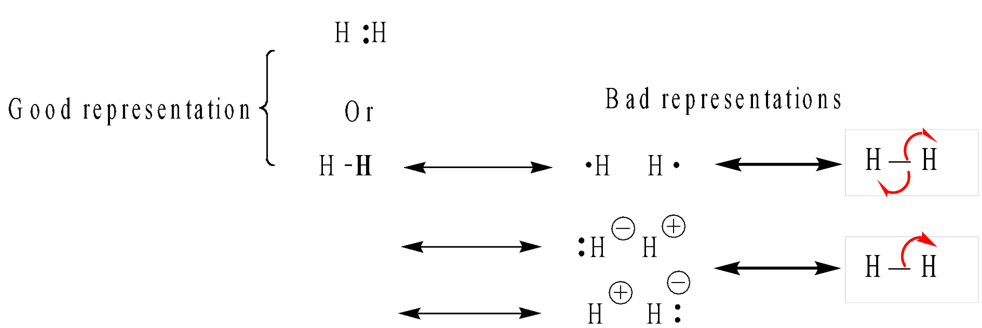


Double Headed Arrow
Show movement of $2e^-$

Fish Hook Arrow
Show movement of $1e^-$

Examples

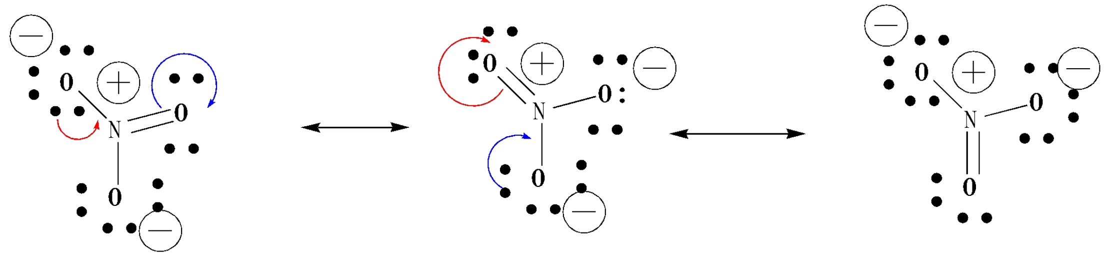
1. Hydrogen gas, H_2



In the bad representations, non- inert gas configuration and extra charges have been created

2. Sodium Nitrate, $NaNO_3$, $Na^+ NO_3^-$

(Nitrate has 3 resonance forms shown here)

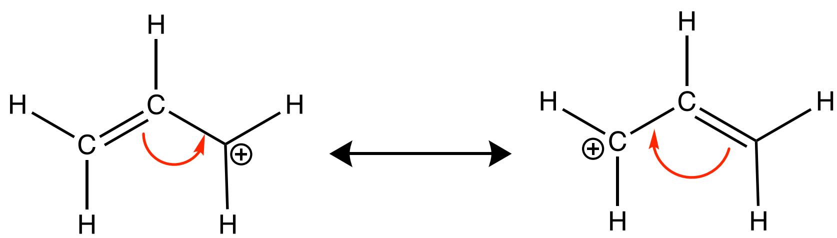


No inert gas configuration disrupted

No extra charge created

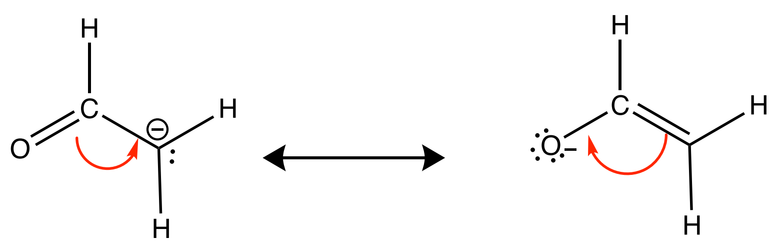
- The O atoms contain partial single and double bond characteristics (each O has -2/3 charge)

3. Allyl Cation



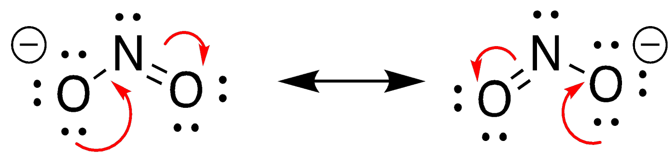
-electrons are delocalized between the two carbons on both side of the central C and C atoms has -1/2 charge and contains partial double and single bond character.

4. Keto-Enol



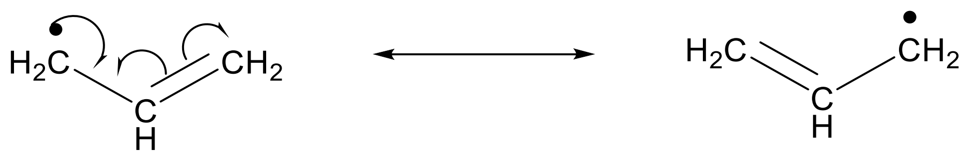
Ketone **Enolate**

5. Sodium Nitrite, $NaNO_2$



Nitrite anion is reactive in both O atoms. Electrons are delocalized in more than one atom – both O atoms has -1/2 charge and contains partial double and single bond character.

6. Allyl Radical

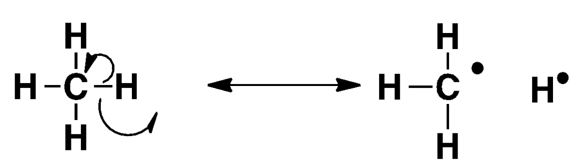


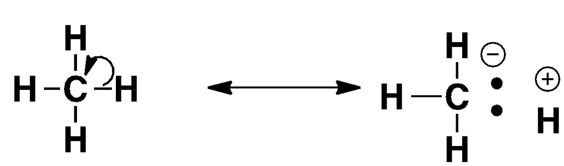
The radical is relatively stable due to resonance.

7. Propyne cation

8. CH_4 Methane – below are **POOR** resonance structures – additional charges or unshared electrons (not inert gas configuration)

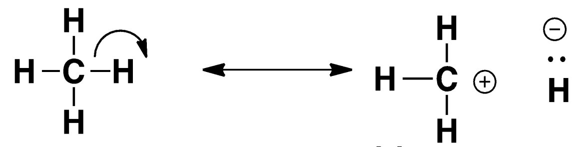
but methyl radical – can be reactive intermediate in principle



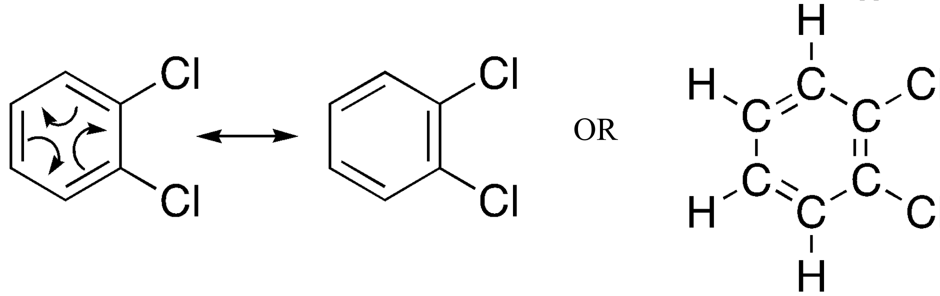


but methyl anion – can be a reactive intermediate in principle

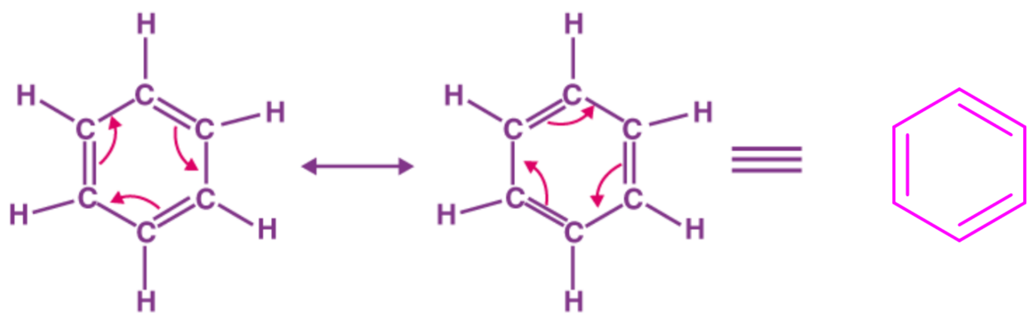
but methyl cation – can be a reactive intermediate in principle



9. 1,2-Dichlorobenzene



8. Benzene



Intermolecular Forces: (forces present between molecules)

- Attractive intermolecular forces:
  i) **Hydrogen bonding** – strongest on per atom basis (e.g. base recognition in forming DNA helix) (also in RNA)
     - *Linus Pauling - development of H bonding*
  ii) **Dipole-dipole interaction** (Intermediate strength)
  iii) **London forces** (temporary dipole; hydrophobic bonding) – weakest on per atom basis – distortion of inner shells.

Electronegativity:

- An atom's desire for electrons (negative charge).
- On the periodic table, electronegativity increases as you go from left to right (up to inert gases, which are not electronegative) and as you go from down to up
- Halogens (F, Cl, Br, I) are highly electronegative
  - i.e. Fluorine is the most electronegative atom (wants to gain the inert gas configuration of Ne) and is small (has few electrons)

- It influences acidity of H's attached, as well as the intermolecular forces between molecules.

Hydrogen Bonding:

- Strongest intermolecular attractive force
- Need H directly attached to a very electronegative atom (N, O, F, Cl, Br, I)
    - Known as **donors**
- Very electronegative atom needs a lone pair of electrons (N, O, F, Cl, Br, I)
    - Known as **acceptors**