AS A REMINDER:

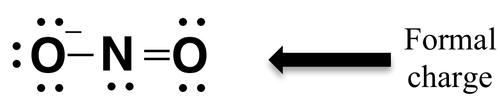
Formal Charge

- 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

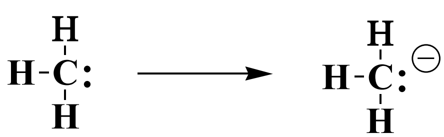
1. **Nitrite anion**



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

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

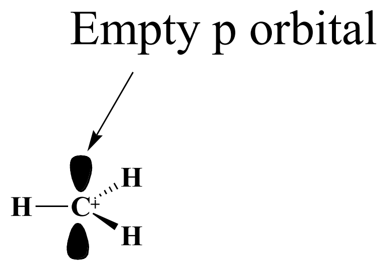
2. **Methyl anion**

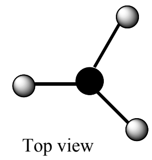


Formal Charge on Carbon
+6 (number of protons)
-2 (1s electrons)
-2 (unshared electrons)
½ x 6 = -3 (1/2 of shared electrons)
-1

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

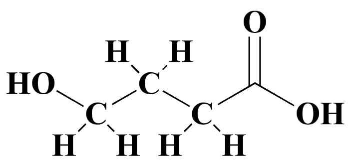
Formal Charge on Carbon
+6 (number of protons)
-2 (1s electrons)
0 (unshared electrons)
½ x 6 = -3 (1/2 of shared electrons)
+1



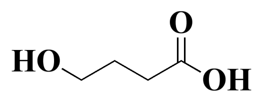


DRAWING CHEMICAL STRUCTURES

γ -Hydroxybutyric acid



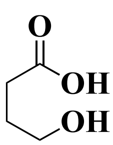
Open chain form

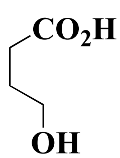


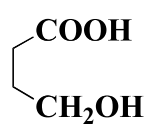
Bond line form

MF = $C_4H_8O_3$

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







Resonance Structures: Different drawings of the same molecule.

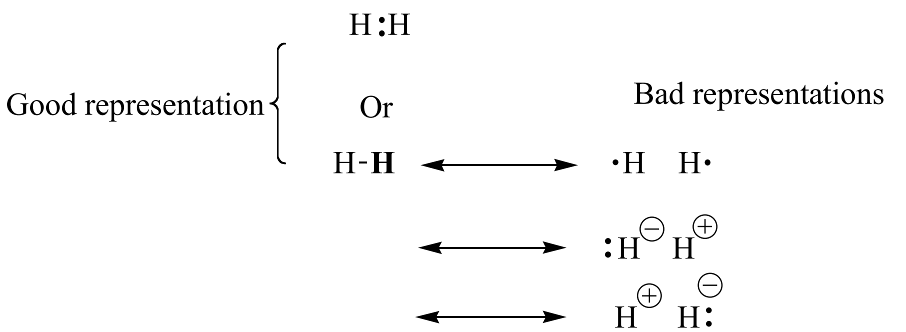
- Move the electrons, keeping the position of the atoms same
- Maintain inert gas configuration around each atom
- Avoid separation of charges
- Avoid like-charges on adjacent atoms
- Double headed arrow (⟷) is used indicate resonance forms

RULES

- Do not create extra charge
- Do not create a non-inert gas configuration

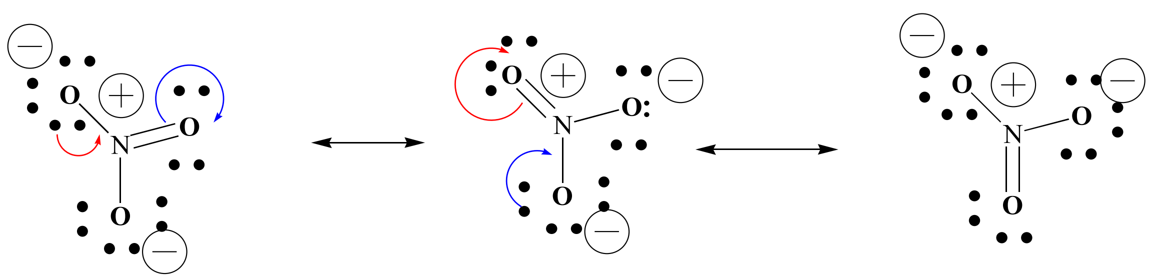
Examples

1. **Hydrogen gas, H_2**



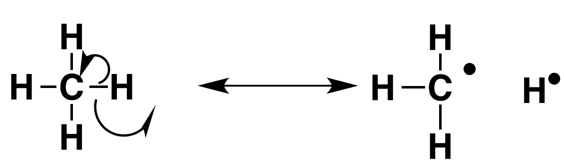
NB: In the bad representations, non- inert gas configuration and extra charges have been created

2. **Sodium Nitrate, $NaNO_3$**

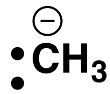


NB: No inert gas configuration created
No extra charge created

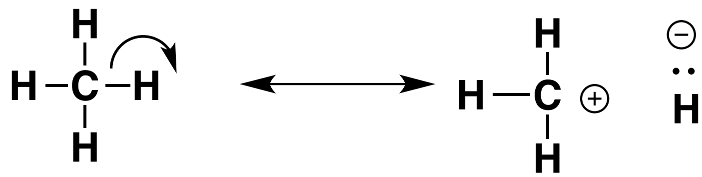
4. **CH_4 Methane** – below are **POOR** resonance structures – additional charges or unshared electrons (not inert gas configuration)



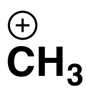
but methyl radical – can be
reactive intermediate in principle



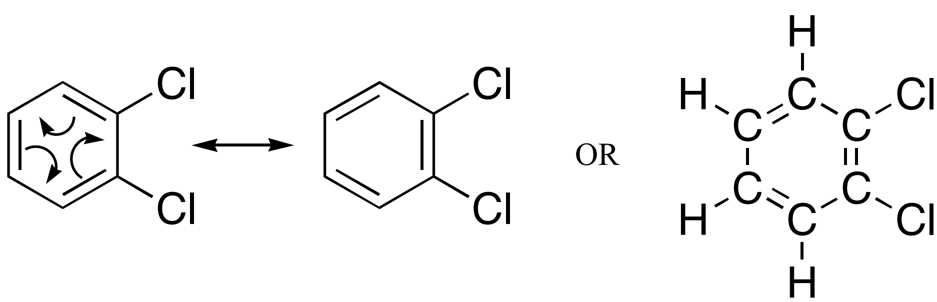
but methyl anion – can be a reactive
intermediate in principle

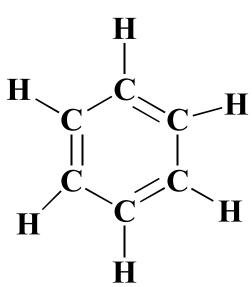


- can be a Methyl cation
- reactive intermediate in principle



5. 1,2-Dichlorobenzene





BENZENE

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
    - 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.

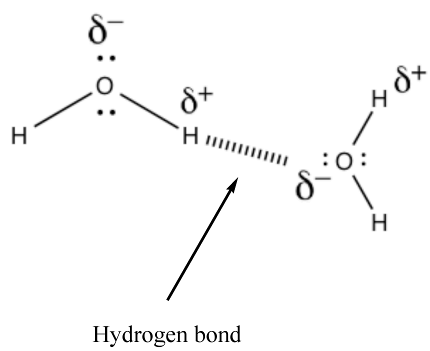
Intermolecular Forces: (forces present between molecules)

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

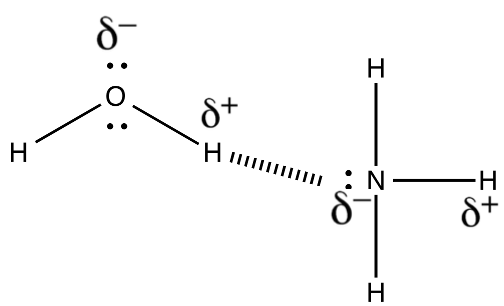
Hydrogen Bonding:

- Donors: H attached to a very electronegative atom (N, O, F, Cl)
- Acceptors: A lone pair of electrons, usually on N or O or F
- Strongest intermolecular attractive force on a per atom basis

e.g. H-O-H (water)



- Oxygen is electronegative and it is sp^3 hybridized
- The partial positive charge on H and the partial negative charge on O lead to their attraction
- Results in high boiling point (100 C) and high melting point by self-association
- HF, H_2O and NH_3 form hydrogen bonds



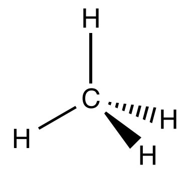
1. Water is a liquid at RT while ammonia is a gas
2. Oxygen is more e-neg than nitrogen, so the protons on water have a higher positive partial charge than the protons on ammonia
3. In an ammonia solution, water would be the hydrogen bond donor and ammonia would be the acceptor
4. Water dissolves ammonia very well – up to 18M

Dipole-Dipole Interactions:

Dipole drawing convention:

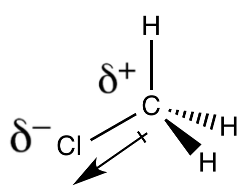
Partial positive charge is the "plus" end, partial negative charge is the arrow head

1. Methane; CH_4



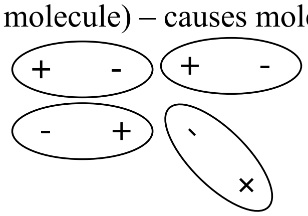
- C and H have ~same electronegativity
- Non-polar (net-zero ~dipole)
- Gaseous
- Low BP -164 ^{o}C (this is relatively low compared to water at 100^{o}C)
- Low MP -182 ^{o}C

2. Chloromethane, methyl chloride; CH_3Cl

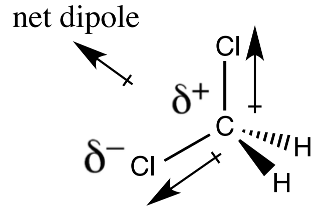


- H and C have similar electronegativity values (non-polar bond)
- Cl is very electronegative due to the fact that it only needs one electron to get inert gas configuration.
- Electron density is pulled toward the chlorine atom, creating a net dipole toward chlorine atom. A net dipole is the vector sum of individual bond dipoles.

Dipoles in different molecules tend to line-up temporarily with each other (partial positive / negative charge on the molecule) – causes molecules to "stick" to each other

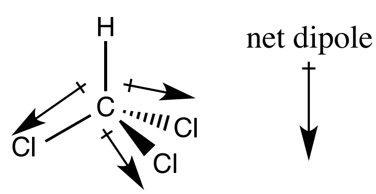


3. Dichloromethane, methylene chloride; CH_2Cl_2



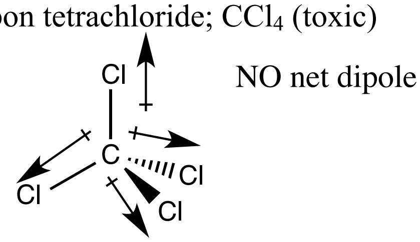
- Liquid at room temperature BP 40 ^oC MP – 95 ^oC
- More polar than chloromethane
- Not miscible with water

4. Trichloromethane, chloroform; $CHCl_3$



- More polar than methylene chloride BP 61 ^oC MP – 64 ^oC

5. Tetrachloromethane, carbon tetrachloride; CCl_4 (toxic)

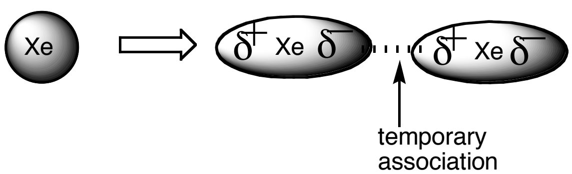


- Non-polar molecule (net-zero dipole)
- Has temporary dipoles since chlorine is polarizable (see below), BP ~77
- Historically used as a dry cleaning fluid

London Forces (Temporary Dipoles):

- Also know as London dispersion forces
- Distortion of filled outer shell electrons
- Principal effect in hydrophobic interactions

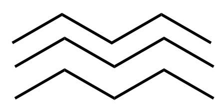
Atoms	Boiling Point	
He	-269 ^{o}C	Small atom/ Low polarizability
Ne	-246 ^{o}C	↓
Ar	-186 ^{o}C	
Kr	-153 ^{o}C	
Xe	-108 ^{o}C	Large atom/ High polarizability



- The larger the atom (expanded electron density), the easier the formation of temporary dipoles

CH_4 associates with CH_4 due to London forces
C_5H_{12} hydrophobic bonding

$H_3C-CH_2-CH_2\cdot CH_2-CH_3$ n-pentane
n= Normal=straight



n-pentane is a liquid at 20^{o} C - why is it a liquid? Because its temporary dipoles – it is not miscible in water – water would rather hydrogen bond to itself – like dissolves like
-