Formal Charge

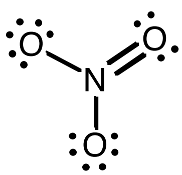
- Convention to keep track of charges
- ∑ (sum of) of formal charges = charge on molecule

Rules

- 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

Formal charge on N calculation

ex)

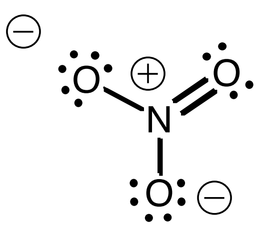


Nitrate

+7 protons in nucleus
-2 (1s electrons)
0 (unshared electrons)
(1/2 x 8) = -4 (1/2 unshared electrons)
+1

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

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

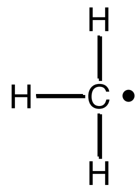


Nitrate

Overall Charge is -1

Formal charge on C:

ex)

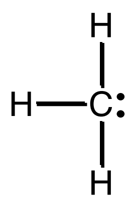


+6 (protons in nucleus)
-2 (1s electrons)
-1 (unshared electrons)
(1/2 x 6) = -3 (1/2 unshared electrons)
0

This species is called methyl radical – not stable.

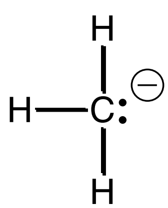
Formal charge on C:

ex)



+6
-2 (1s electrons)
-2 (unshared electrons)
(1/2 x 6) = -3 (1/2 unshared electrons)
-1

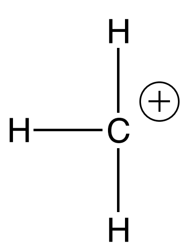
This species is called methyl anion and could be written as:



Isoelectronic with Ne, but also not stable.

Formal charge on C:

ex)



+6
-2 (1s electrons)
-2 (unshared electrons)
0 unshared electrons)
+1

This species in methyl cation, and is even less stable than methyl anion.

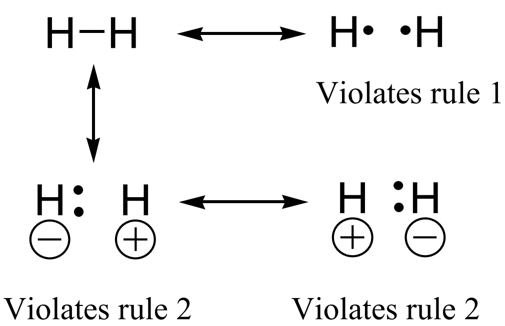
Resonance Structures:

- Give different pictures of the same molecule, they are made by moving electrons and keeping the position of the atoms same.

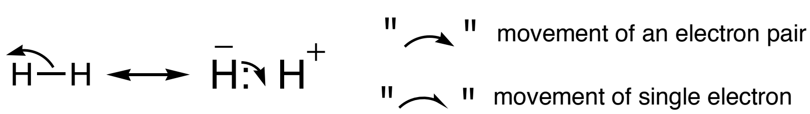
Rules for good resonance structures

1) maintain inert gas configuration around each atom
2) avoid generation of additional charges
3) avoid like-charges on adjacent atoms

Eg. Hydrogen gas, H_2:



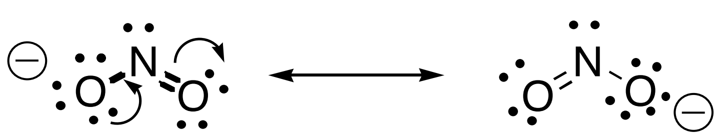
- they are all resonance forms but not necessarily good ones (accurate)
- H-H is the best resonance form
- Double headed arrow ($\longleftrightarrow$) is used to indicate resonance forms



* this is called "arrow pushing" → bookkeeping of electrons

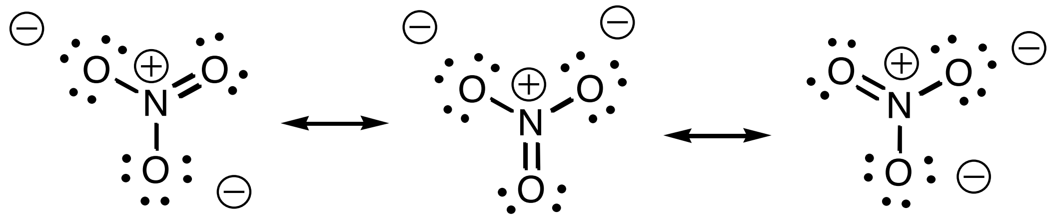
Resonance structure:

1. nitrite anion (NO_2^-)



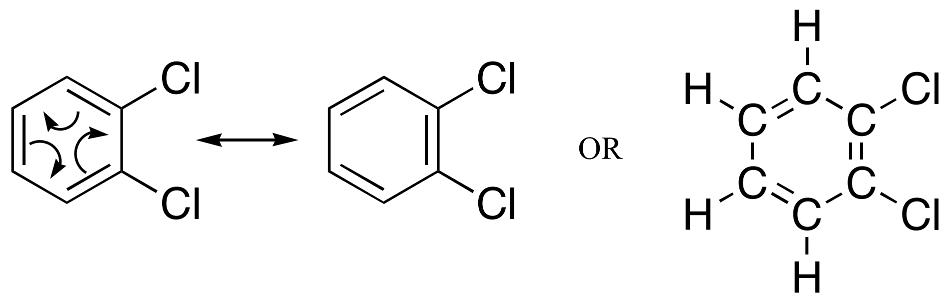
The two resonance structures shown above are equally valid.

2. nitrate anion (NO_3^-)



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

3. $C_6H_4Cl_2$



Intermolecular forces: (forces present between molecules)

- Attractive intermolecular forces:
  - i) Hydrogen bonding – strongest on per atom basis (eg. base recognition in forming DNA helix)
  - ii) Dipole-dipole interaction
  - iii) London forces (temporary dipole) – weakest on per atom basis

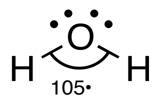
Electronegativity:

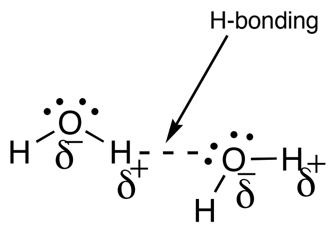
- An atom's desire for electrons (negative charge).
- in Periodic table, electronegativity increases as you go from left to right (up to inert gases which are not electronegative) and as you go upwards
- Eg. Fluorine is the most electronegative atom (wants to gain the inert gas configuration of Ne)

Hydrogen bonding:

- need a lone pair of electrons
- need hydrogen directly attached to a very electronegative atom (F, O, N) for Hydrogen bonding between molecules of same type
- strongest intermolecular attractive force on a per atom basis

eg. H-O-H (water)

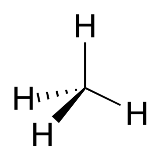




- oxygen is electronegative and it is sp^3 hybridized
- leads to high boiling point and high melting point by self association

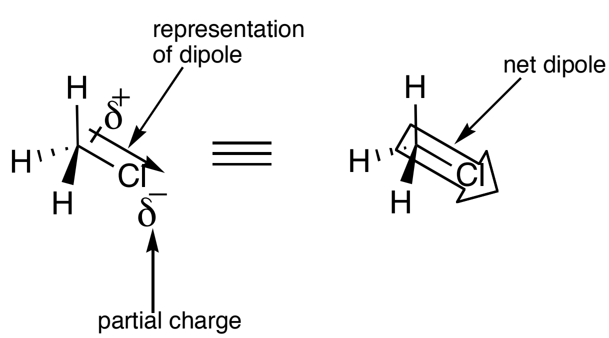
Dipole moment:

Eg.
1. Methane CH_4



- Non-polar (net-zero dipole)
- Gaseous
- Low BP -164 ^oC
- Low MP -182 ^oC

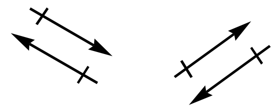
2. Methyl chloride, CH_3Cl, $ClCH_3$



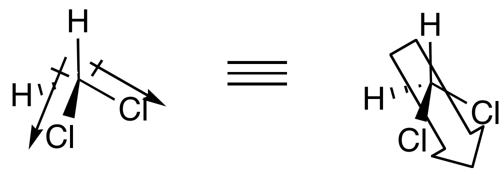
- H and C have similar electronegativity values (non-polar bond)
- Cl is very electronegative – due to the fact that it only needs one electron to get inert gas configuration. (C-Cl and C-F are polar bonds)

- Electron density is pulled towards chlorine atom – so a net dipole toward chlorine atom – 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

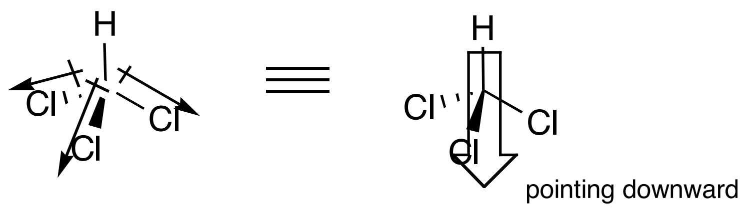


3. Dichloromethane, methylene chloride, CH_2Cl_2



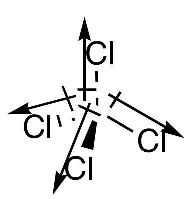
- Liquid at room temperature BP 40 °C MP – 95 °C
- More polar than methyl chloride

4. trichloromethane, chloroform, $CHCl_3$



- More polar than methylene chloride BP 61 °C MP – 64 °C

5. tetrachloromethane, carbon tetrachloride, CCl_4 (TOXIC)

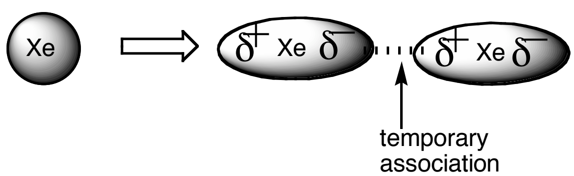


- net-zero dipole

- Non-polar molecule
- Has temporary dipoles and as chlorine is polarizable (see below), high BP

London Forces (temporary dipole):
- also know as dispersion forces
- Principal effect in hydrophobic interaction

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