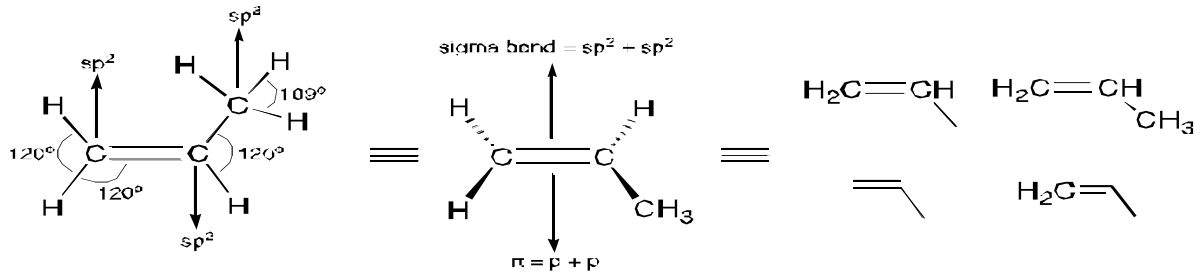
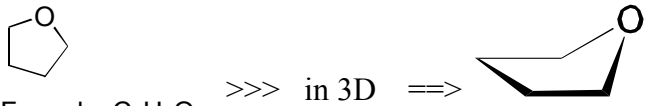
Representation of Molecules

- 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

ex) C_3H_6 (propene)



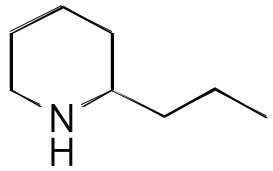
Ex) Tetrahydrofuran (THF)



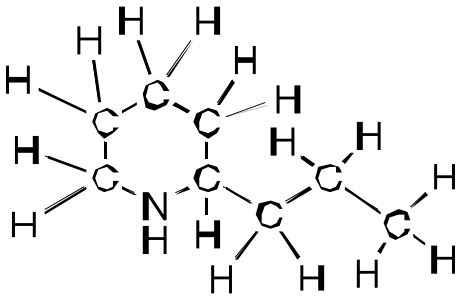
Chemical Formula: C_4H_8O
Molecular Weight: 72.1070

>>> in 3D ==>

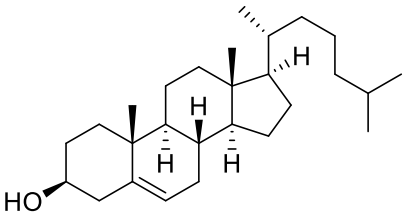
ex)



coniine (poison hemlock)



E.g. Cholesterol:



Chemical Formula: $C_{27}H_{46}O$
Molecular Weight: 386.6640

Formal Charge

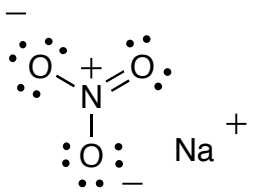
- Convention to keep track of charges
- ∑ (sum of) of formal charges = charge on molecule

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

E.g.

1. **Sodium Nitrate – $NaNO_3$**

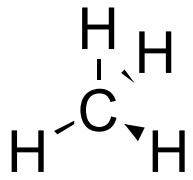


Double bonded oxygen:
+8 (number of protons)
-2 (1s electrons)
-4 (unshared electrons)
½ x 4 = -2 (1/2 of shared electrons)
0

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

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

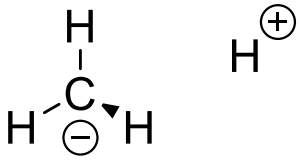
2. Methane:



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 Anion/Carbanion**:

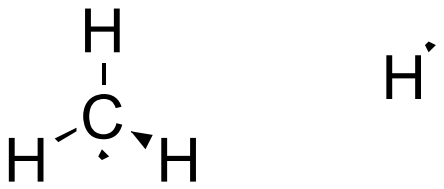


Formal Charge on Carbon:
+6 (number of proton)
-2 (1s electron)
-2 (unshared electrons)
½ x 6 = -3 (1/2 of shared electrons)
-1

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

4) Methyl Radical:

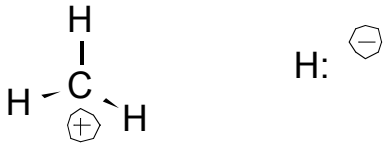


Formal Charge on Carbon:
+6 (number of proton)
-2 (1s electron)
-1 (unshared electrons)
½ x 6 = -3 (1/2 of shared electrons)
0

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

5) Methyl Cation:



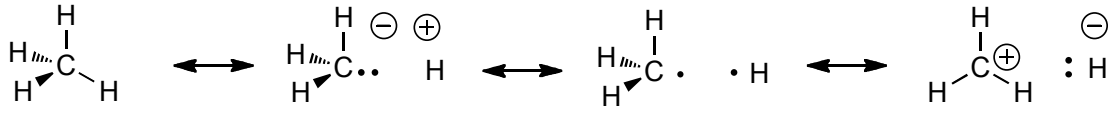
Formal charge on Carbon
+6 (number of protons)
-2 (inner shell e-)
-3 (1/2 shared e-)
_____
+1

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

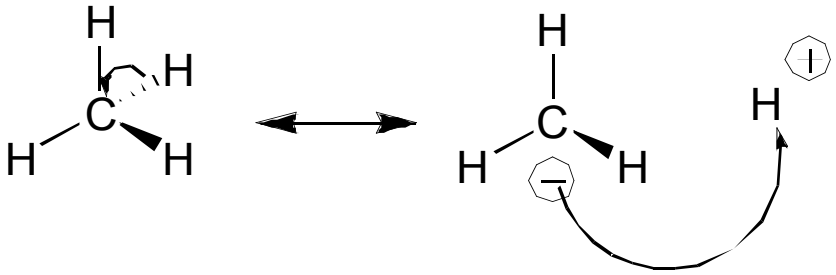
Resonance:

- move the electrons, keeping the position of atoms same → gives different picture of same molecule
- maintain inert gas configuration around each atom
- avoid separation of charges
- avoid like-charges on adjacent atoms

Eg. Methane:



- they are all resonance forms but not necessarily good pictures (significant representations of actual structure
- CH_4 is the best resonance form
- Double headed arrow (⟷) is used indicate resonance forms



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

Resonance structure example:

1. nitrate anion (NO_3^-)