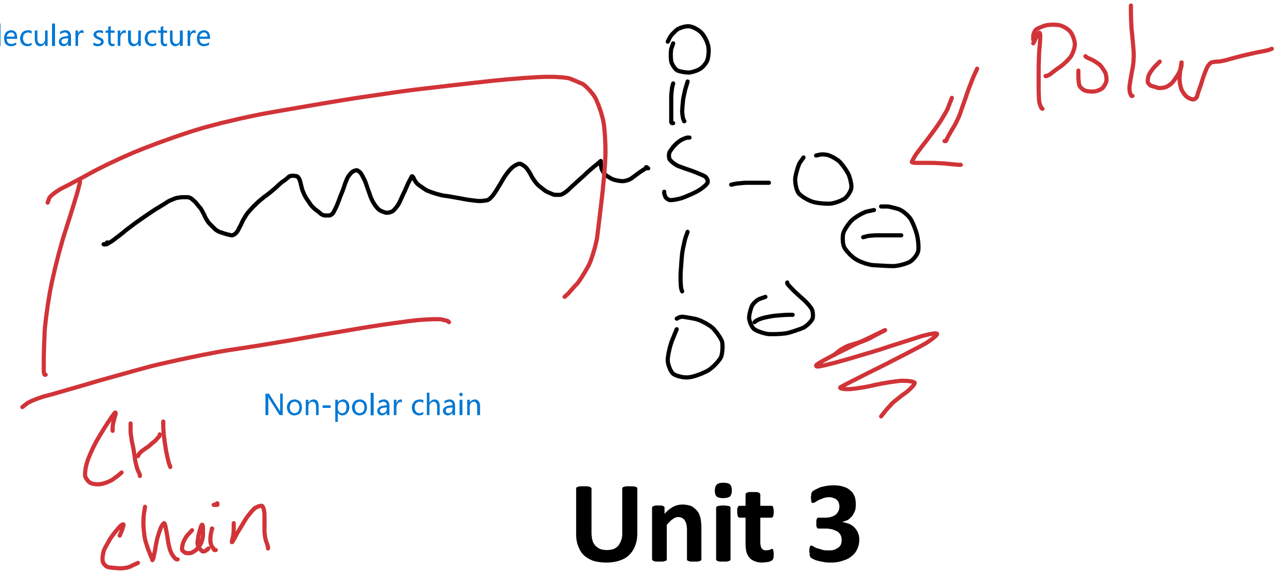
Examples of molecular structure

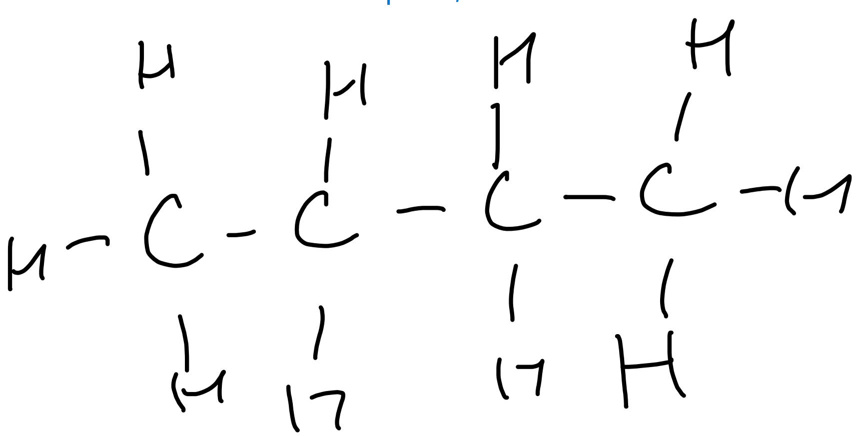


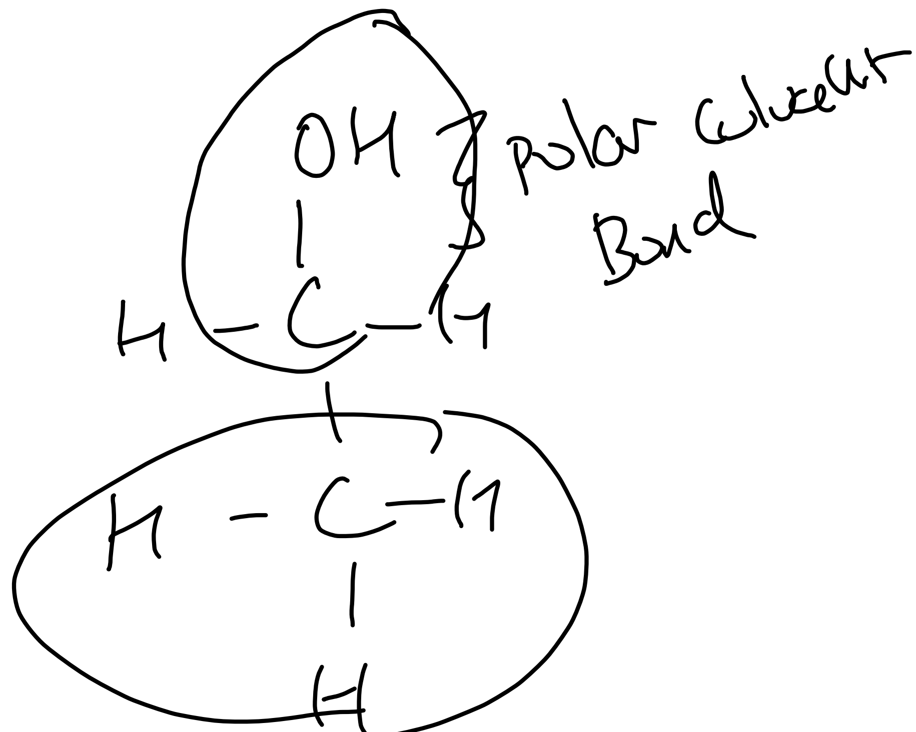
Non-polar chain

Unit 3

Molecular Structure

Non-polar; covalent bond





Blueprint question

https://www.chemistryworld.com/earth/explainer-why-are-chemical-dispersants-used-in-oil-spills/1017322.article

Learning Objectives (Part 1)

After mastering this unit you will be able to:

- Draw Lewis structures for a given chemical formula, or use the features of a Lewis structure to identify the unknown elements or chemical formula of a molecule.
- Draw resonance structures, or identify valid resonance structures, for a given molecule.

Bonding Theories

Molecular Orbital Theory (exact)

- Correct quantum mechanical description with orbitals extending over entire molecule

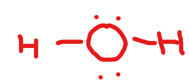
Valence Bond Theory (not quite exact)

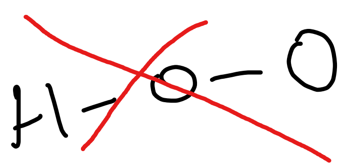
- Localized electron picture with bonds formed by the overlap of singly occupied atomic orbitals

Lewis Theory (approximate)

- Localized electron picture using rules based upon counting electrons

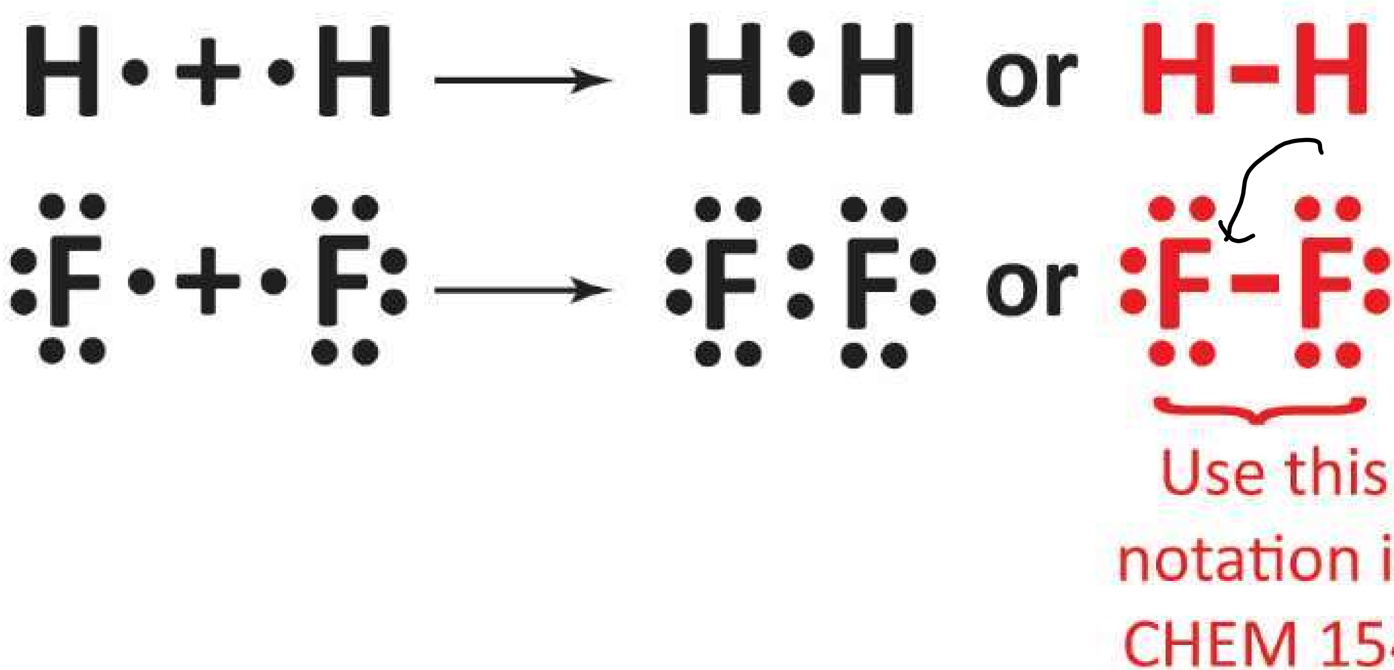
H_2O





Representation of Covalent Bonds

A **Lewis structure** shows how valence electrons are shared in a molecule. Valence electrons that form a bond are called bonding pairs. Valence electrons that do NOT form a bond are called lone pairs.



$2e^-$

$-$ $2e^-$

$=$ $4e^-$

$\equiv$ $6e^-$

KEEP
CALM
AND
DRAW LEWIS
DOT STRUCTURES

Lewis Structures

Octet Rule

In forming chemical bonds, main group elements gain, lose, or share electrons to achieve a configuration in which they are surrounded by 8 valence electrons.

8

Duet Rule

For hydrogen only, surrounded by 2 electrons.

Note: exceptions can happen, e.g. Boron

Drawing Lewis Structures – Formal charge

Formal charge: Formal charge is the difference between the number of valence electrons and the number of electrons surrounding an atom in a particular Lewis structure.

Consider why high chargers are unlikely.

$^{+4}C - N^{-4}$

$9 \cdot 10^9$

$\frac{K q_1 q_2}{r^2}$

$$FC = VE - LPE - 1/2(BE)$$

VE = number of valence electrons

LPE = number of lone pair electrons

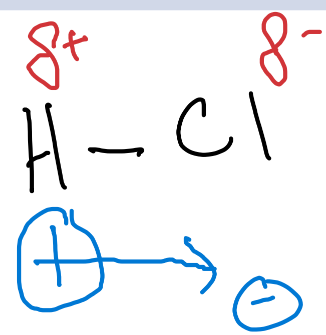
BE = number of bonding electrons

The overall molecular charge is the SUM of the formal charges.

Electron Bookkeeping and Reality

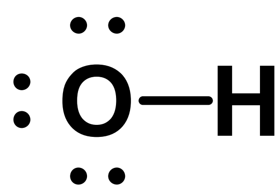
Several different methods are used in chemistry for electron bookkeeping, each with their own particular application and philosophy. The table below contrasts formal charges and oxidation states with reality for the molecule HCl.

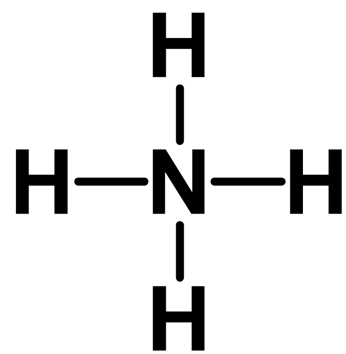
Method	Charge on H	Charge on Cl	Description
Formal Charge	0	0	Bonding e^- shared equally
Oxidation State	+1	-1	Bonding e^- to atom with highest EN
Reality	δ^+	δ^-	Polarized bonds with fractional charges

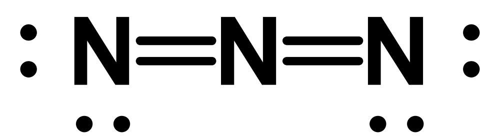


Worksheet Question #1

Calculate the formal charge of each atom in the following structures:





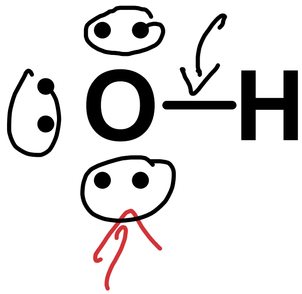


The overall molecular charge is NOT given in these structures. It is the SUM of the formal charges!

Worksheet Question #1

Calculate the formal charge of each atom in the following structures:

$VE - LPE - \frac{1}{2}(BE)$



$1 - 0 - \frac{1}{2}(2)$

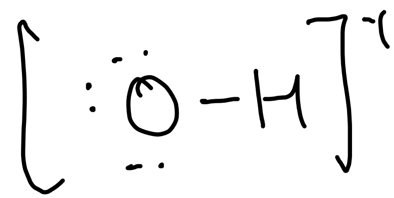
$1 - 0 - 1$

$= 0$

$6 - 6 - \frac{1}{2}(2)$

$0 - 1$

$= -1$

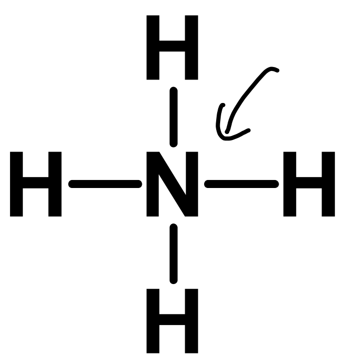


NaOH

Worksheet Question #1

Calculate the formal charge of each atom in the following structures:

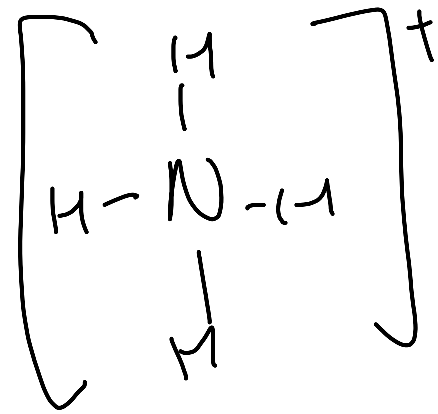
B C N O F Ne
3 4 5 6 7 /

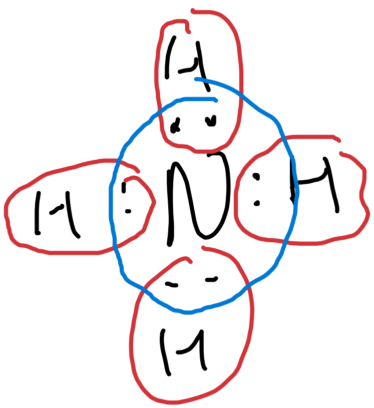


$5 - 0 - \frac{1}{2}(8)$

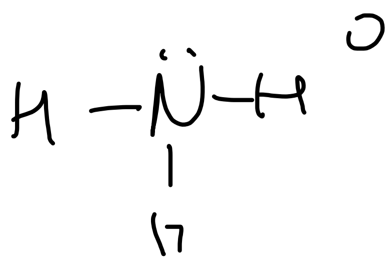
$5 - 4$

$= 1$





Bonding electrons for each atom encircled.



Worksheet Question #1

The formal charges in the nitrogen atoms in the azide below are:

NaN_3

$+1$

$:\ddot{N}=N=\ddot{N}:$

1 2 3

A

$VE - LPE - \frac{1}{2}(BE)$

$5 - 0 - \frac{1}{2}(8) = 1$

$5 - 4 - \frac{1}{2}(4) = -1$

$:N \equiv N:$

	N_1	N_2	N_3
A	0	0	0
B	0	+1	0
C	-1	0	-1
D	-1	+1	-1
E	None of the above		

Drawing Lewis Structures

1. Count the number of valence electrons (#ve$^-$) in the molecule or ion
2. Draw the skeletal structure of the molecule
   a) The least electronegative atom is generally the central atom
   b) Hydrogen is ALWAYS a terminal atom
   c) Unless told otherwise, do NOT form rings
3. Place two electrons in each bond of the skeletal structure (represented by single lines)

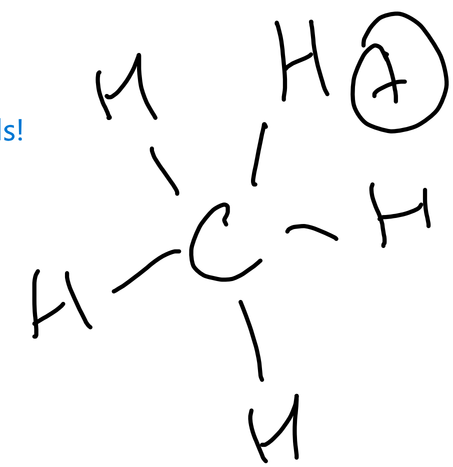
Drawing Lewis Structures

4. Place the remaining valence electrons not accounted for in Step 3 as lone pairs on individual atoms until the octet rule is satisfied
5. Form multiple bonds as needed to complete octets and account for all valence electrons
6. Label the formal charges (FCs)
   - The sum of FCs is equal to the overall molecular charge.

Remember

- Hydrogen atoms are always terminal
- The most stable Lewis structure is the one with the least non-zero formal charges
- The most stable Lewis structure is the one that, when possible, places the negative charge on the most electronegative atom and the positive charge on the least electronegative atom

No carbon with >4 bonds!



Texas Carbon

Lewis Structure Tips

Carbon – always has 4 bonds and no lone pairs

Hydrogen – always has 1 bond

Oxygen – has 2 bonds + 2 lone pairs if FC = 0, 1 bond + 3 lone pairs if FC = -1, and 3 bonds + 1 lone pair if FC = +1 (rare)

Nitrogen – has 3 bonds + 1 lone pair if FC = 0, 4 bonds + 0 lone pairs if FC = +1

These patterns also apply to other elements in the same groups (unless hypervalency is used).