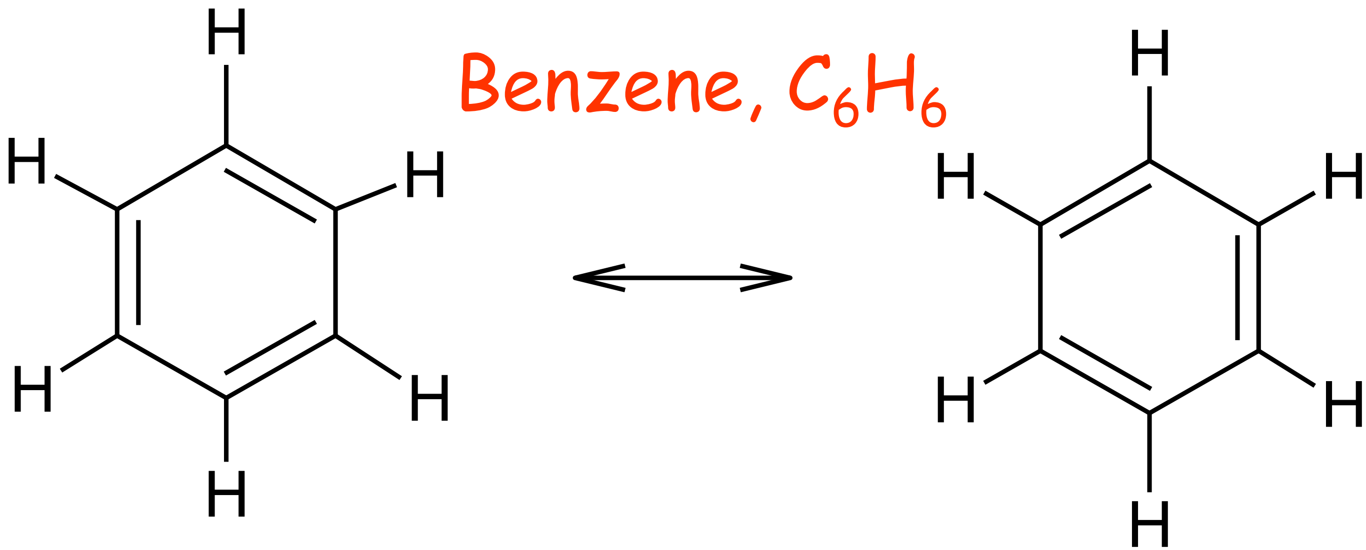
Bonding – General Concepts

FC, VSEPR

Resonance

- Resonance is invoked when more than one valid Lewis structure can be written for a particular molecule.

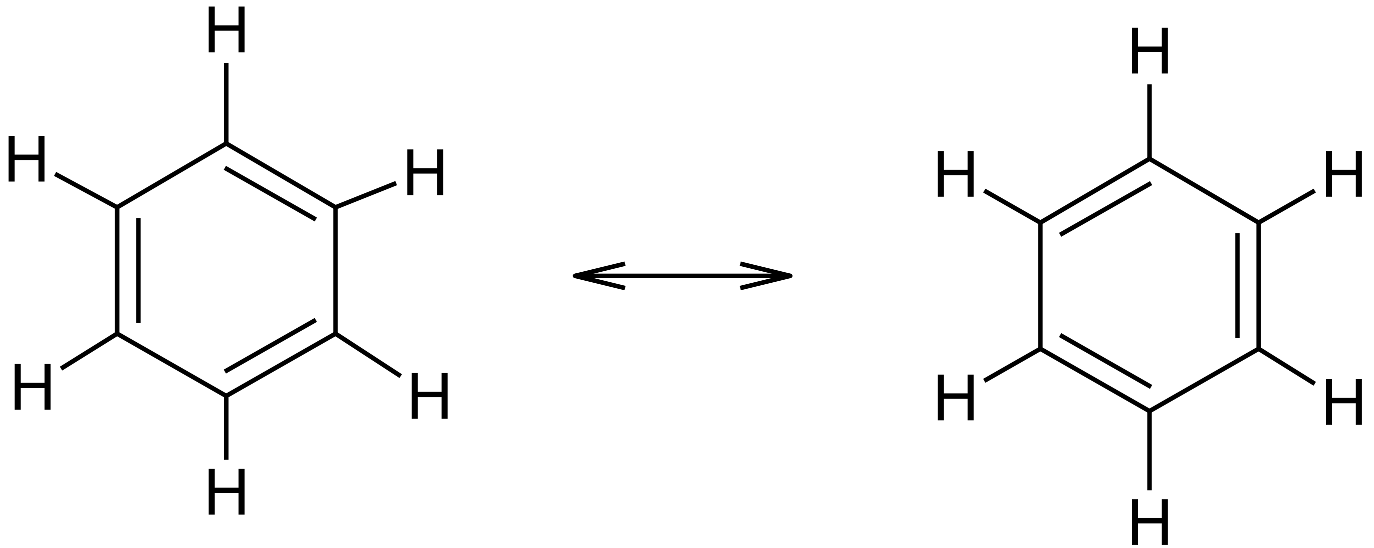
Benzene, C_6H_6



- The actual structure is an average of the resonance structures.
- The bond lengths in the ring are identical, and between those of single and double bonds.

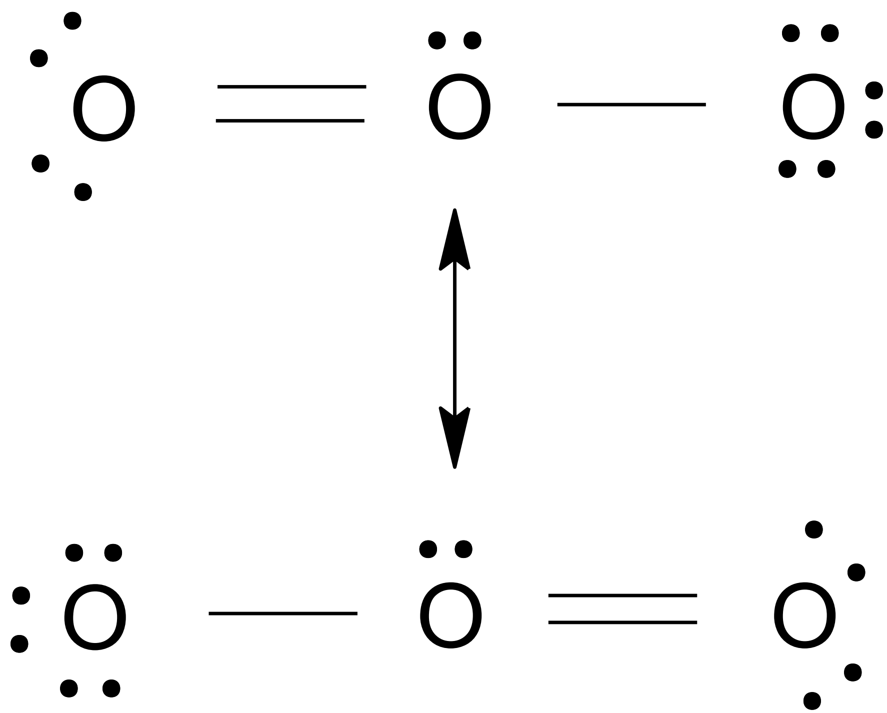
Resonance Bond Length and Bond Energy

- Resonance bonds are shorter and stronger than single bonds.



- Resonance bonds are longer and weaker than double bonds.

Resonance in Ozone, O_3

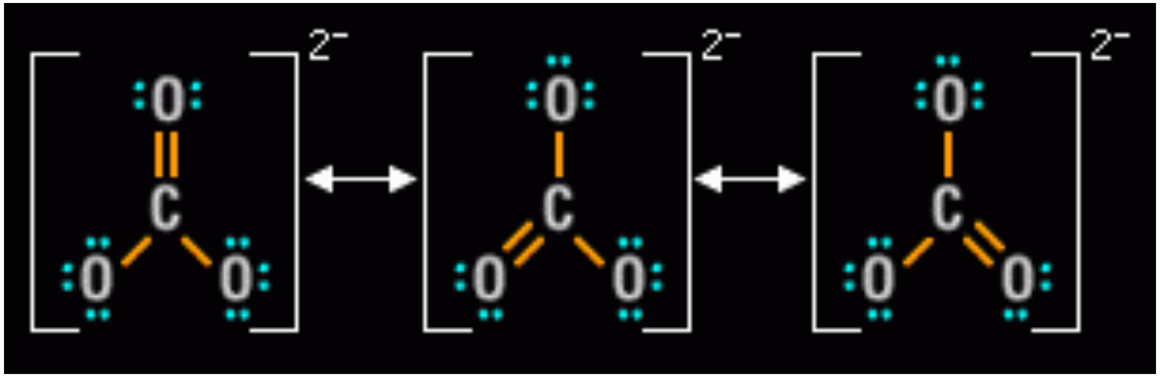


Neither structure is correct.

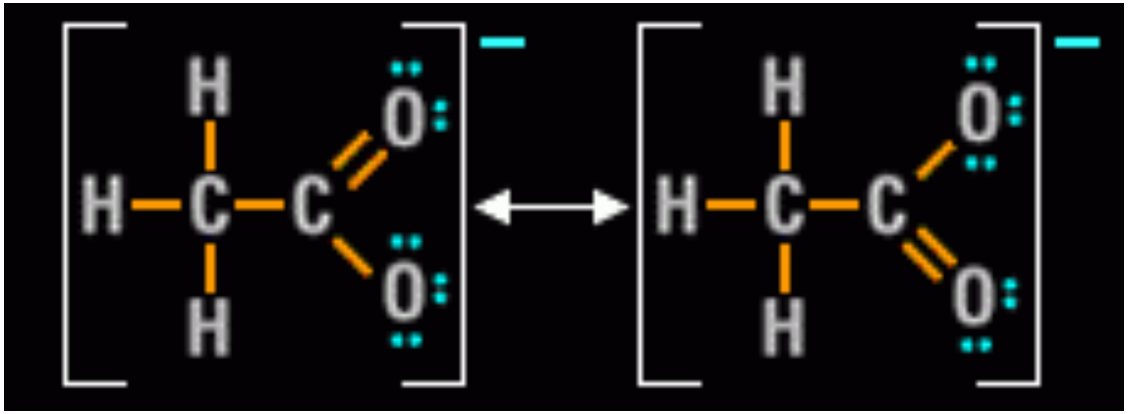
Oxygen bond lengths are identical, and intermediate to single and double bonds

Resonance in Polyatomic Ions

Resonance in a carbonate ion:



Resonance in an acetate ion:



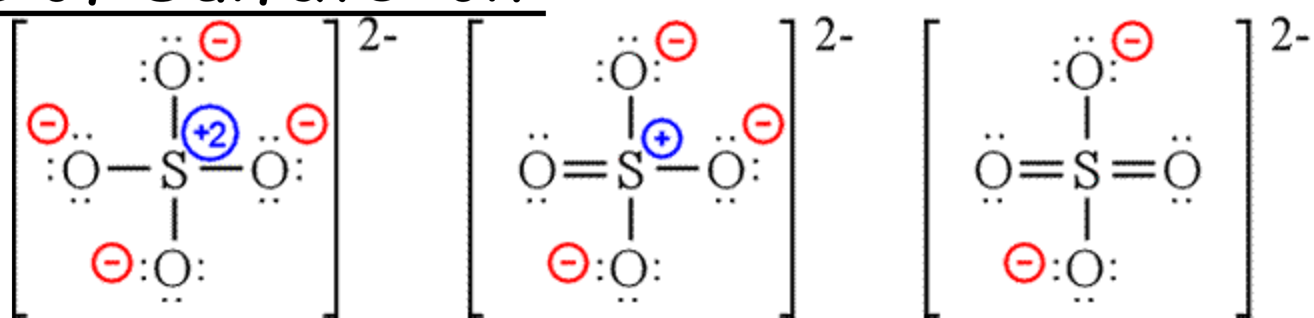
Resonance with FORMAL CHARGES

Equation:

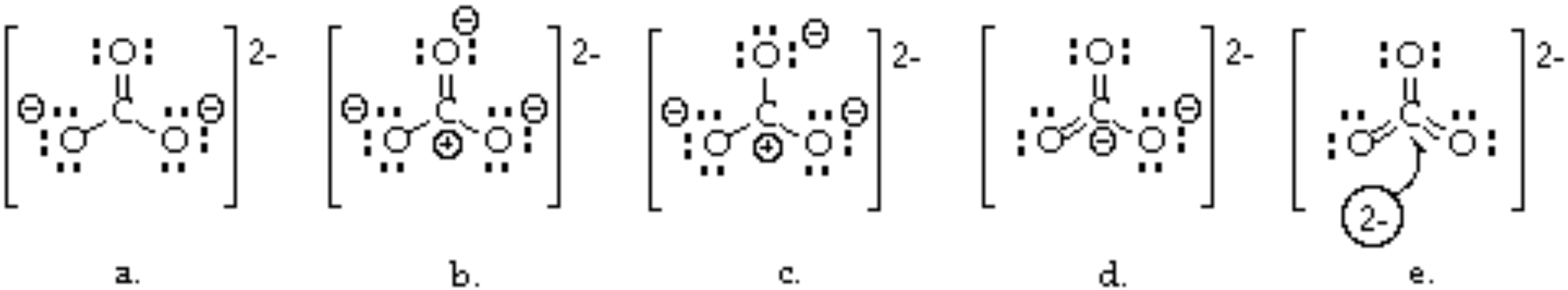
$$\text{Formal Charge} = \text{Valence Electrons in Neutral Atom} - \left(\text{Unshared Valence Electrons} + \text{Half of the Shared Electrons} \right)$$

- To evaluate a Lewis Structure:
    - Atoms in molecules try to achieve FC as close to zero as possible
    - Any negative FC's are expected to be on the most electronegative atoms
- The Σ of the FC of all atoms must = the overall charge of the ion or molecule

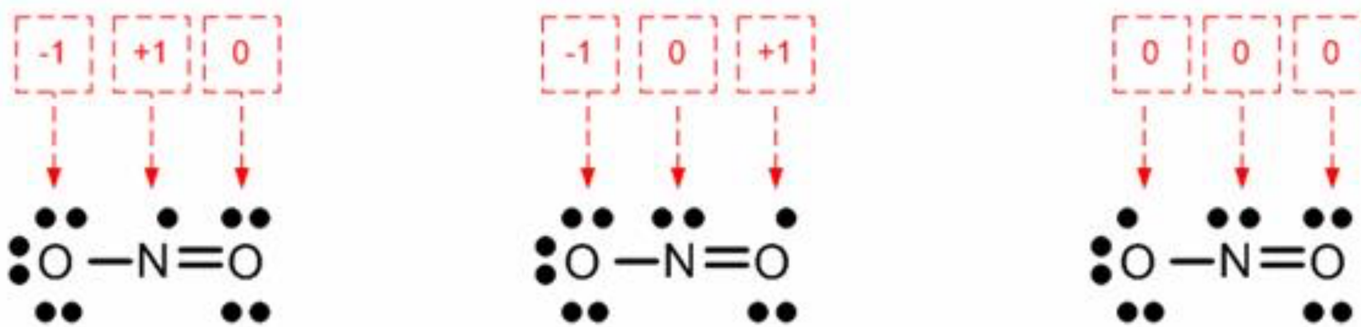
<u>Example of Sulfate ion:</u>



Carbonate Ion



Nitrogen Dioxide



Three possible Lewis structures for nitrogen dioxide. To find formal charges, count non-bonding electrons and one electron for each bond. Subtract the electron count from the valence to get the formal charge. The best Lewis structure (far right) has all atoms' formal charges as close as possible to zero.

Localized Electron Model

Lewis structures are an application of the "Localized Electron Model"

L.E.M. says: Electron pairs can be thought of as "belonging" to pairs of atoms when bonding using atomic orbitals. Lone pairs belong to only one atom

Resonance points out a weakness in the Localized Electron Model.

- What about Delocalized electrons?

VSEPR Model

(Valence Shell Electron Pair Repulsion)

- **The structure around a given atom is determined *principally* by minimizing electron pair repulsions.**

Predicting a VSEPR Structure

- Draw Lewis structure.
- Put pairs as far apart as possible.
- Determine positions of atoms from the way electron pairs are shared
- Determine the name of molecular structure from positions of the atoms using the AXE formula (next slide).

VSEPR – AXE Method

- The A represents the central atom.
- The X represents how many sigma bonds are formed between the central atoms and outside atoms. Multiple covalent bonds (π, double or triple) count as one X.
- The E represents the number of lone electron pairs present on the central atom.
- The sum of X and E, sometimes known as the steric number.

VSEPR – Valence Shell Electron Pair Repulsion

X + E	Overall Structure (Electronic Geometry)	Forms
2	Linear	AX_2
3	Trigonal Planar	AX_3, AX_2E
4	Tetrahedral	AX_4, AX_3E, AX_2E_2
5	Trigonal bipyramidal	AX_5, AX_4E, AX_3E_2, AX_2E_3
6	Octahedral	AX_6, AX_5E, AX_4E_2

A = central atom

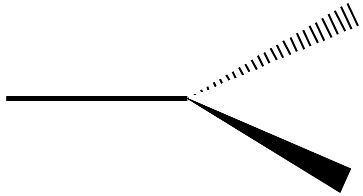
X = atoms bonded to A

E = nonbonding electron pairs on A

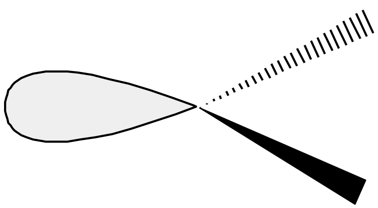
VSEPR: Linear (180°)

__________ AX_2 CO_2 

VSEPR: Trigonal Planar (120°)



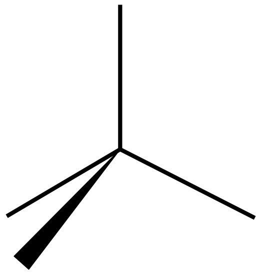
AX_3 BF_3



AX_2E (Bent) $SnCl_2$

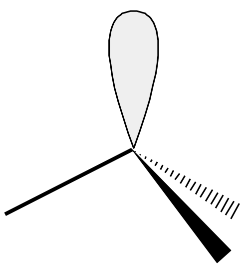
RED = Molecular Geo.

VSEPR: Tetrahedral (109.5°)



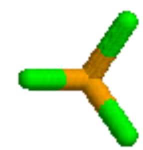
AX_4 CCl_4

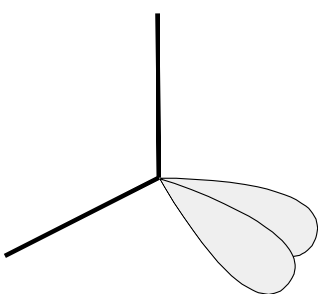
RED = Molecular Geo.



AX_3E (107.5°) PCl_3

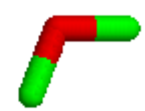
(**Trigonal Pyramidal**)



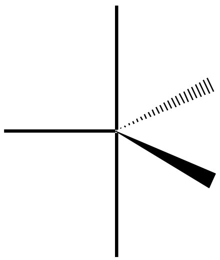


AX_2E_2(104.5°) Cl_2O

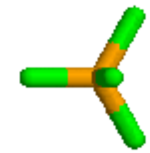
(**Bent**)

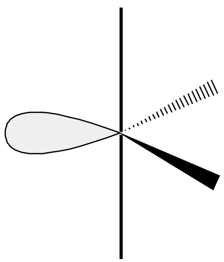


VSEPR: Trigonal Bi-pyramidal (90°,120°)

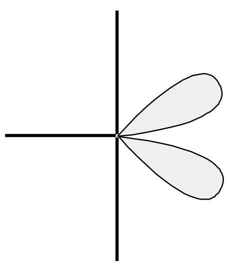


AX_5 — PCl_5

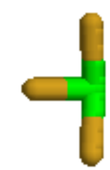


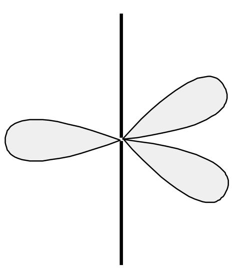


AX_4E (See saw) (180°, 120°) — SF_4



AX_3E_2 (T-shape) (90°, 180°) — ClF_3

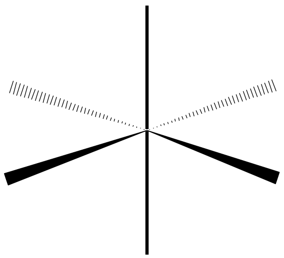




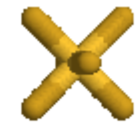
AX_2E_3 (Linear) — I_3^-

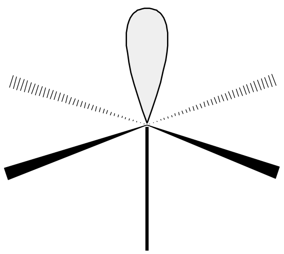
RED = Molecular Geo.

VSEPR: Octahedral (90°)



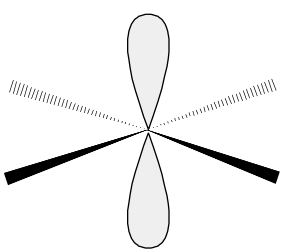
AX_6 SF_6





AX_5E (< 90°) BrF_5

(Square pyramidal)



AX_4E_2 (90°) ICl_4-

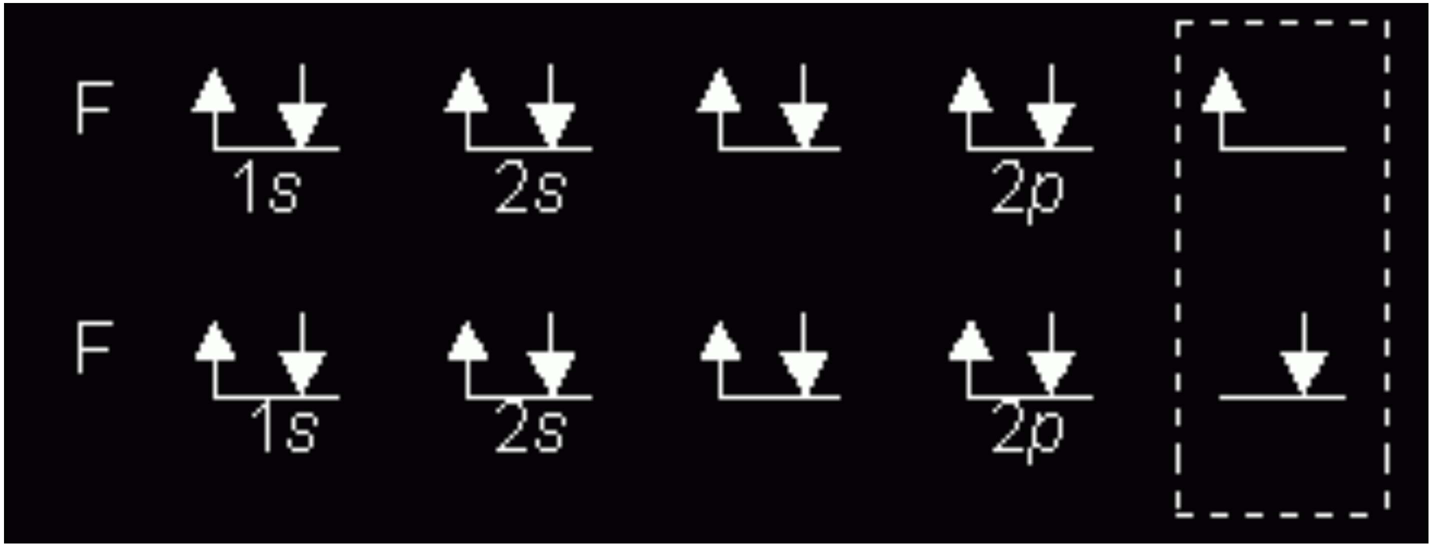
(Square Planar)

RED = Molecular Geo.

REMINDER:
The Octet Rule

Combinations of elements tend to form so that each atom, by gaining, losing, or sharing electrons, has an octet of electrons in its highest occupied energy level.

Diatomic Fluorine



Comments About the Octet Rule

- 2nd period elements C, N, O, F observe the octet rule (HONC rule as well).

Comments About the Octet Rule

- 2nd period elements B and Be often have fewer than 8 electrons around themselves - they are very reactive.

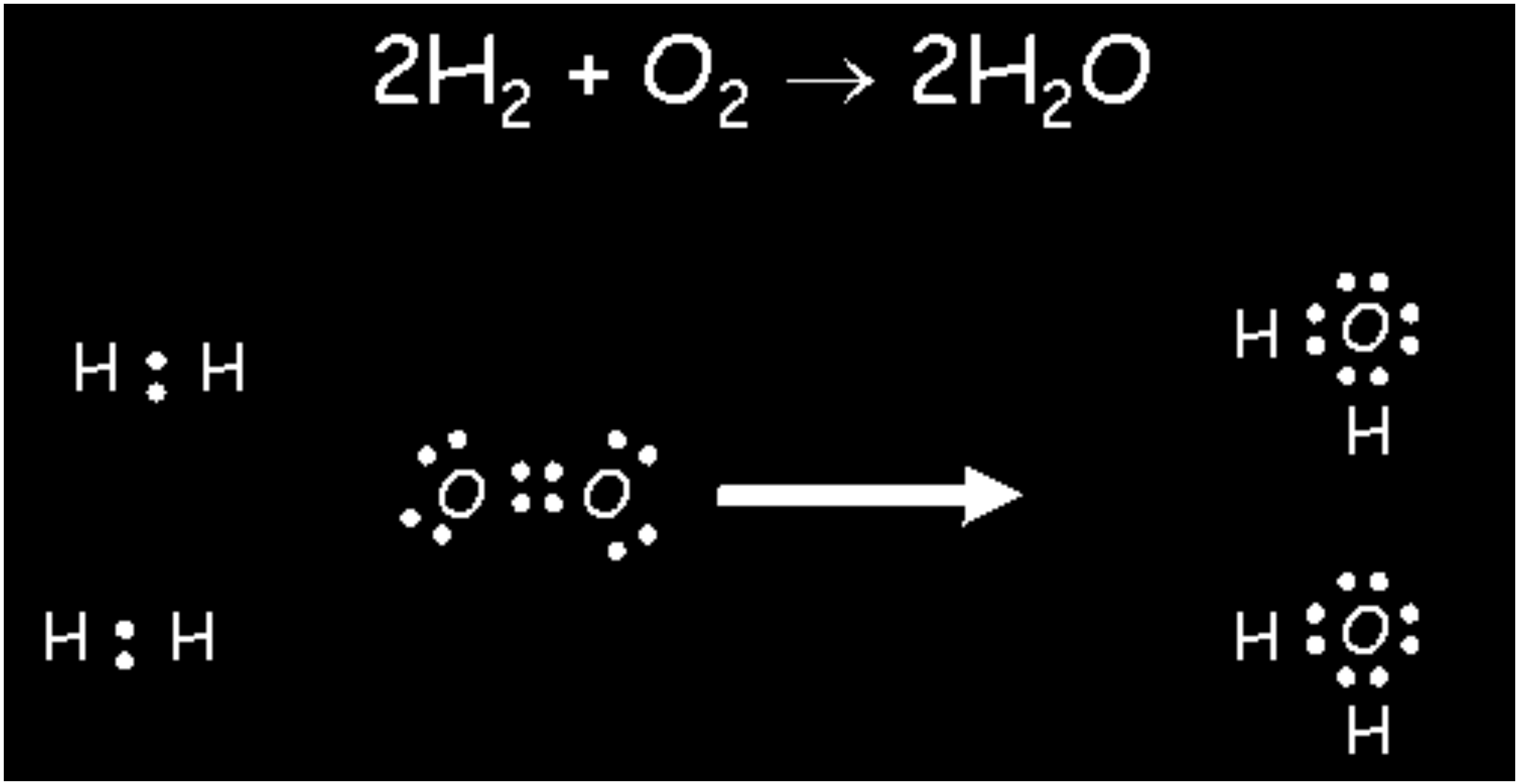
Comments About the Octet Rule

- 3rd period and heavier elements CAN exceed the octet rule having expanded octets (using ?).

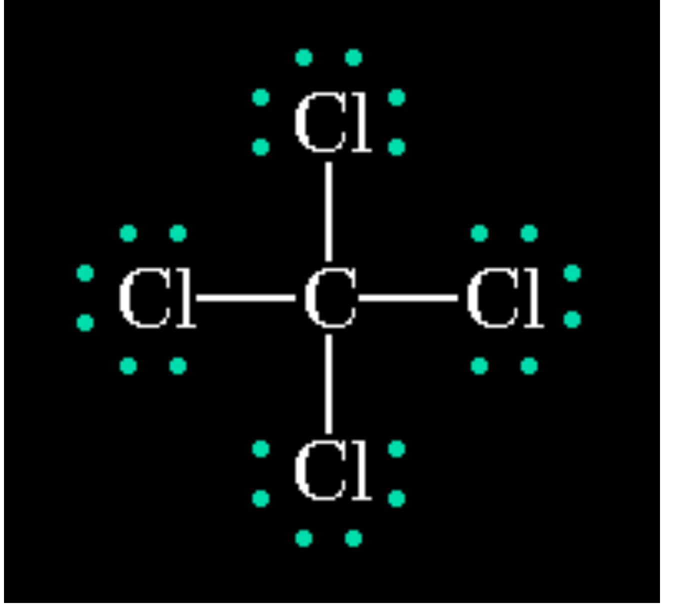
Comments About the Octet Rule

- When writing Lewis structures, satisfy octets first, then place extra electrons around central element if needed

Formation of Water by the Octet Rule



Lewis Structures

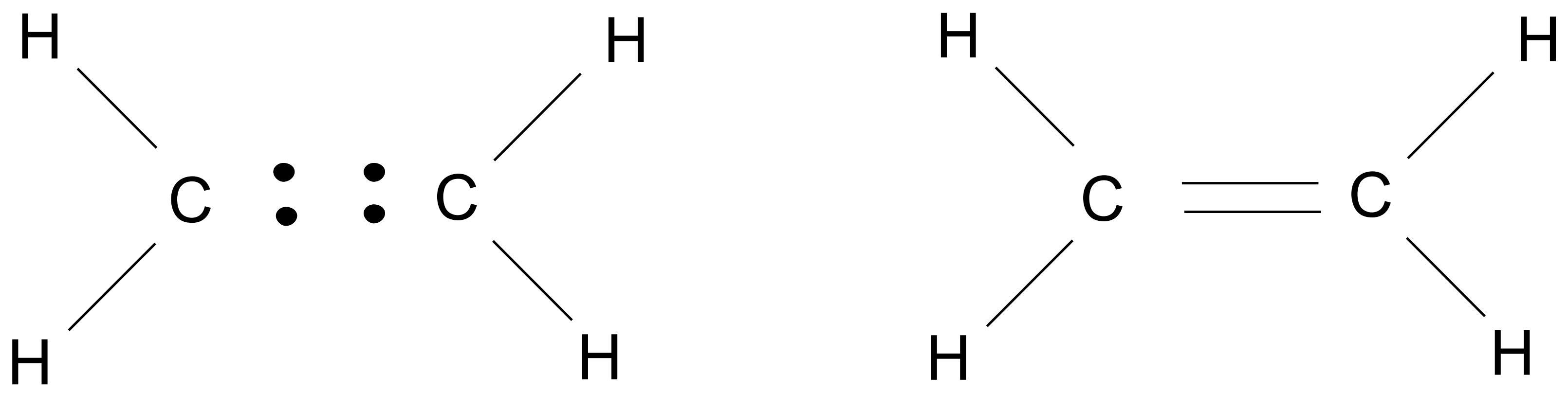


- Shows how valence electrons are arranged among atoms in a molecule.
- Reflects central idea that stability of a compound relates to noble gas electron configuration.

Rules for Drawing Lewis Structures

1. Add up total number of Ve^- and divide by 2 (this =s the number of pairs)
2. The least electronegative atom tends to be your "central" atom
3. Place all other atoms around your central atom
   1. H are always terminal
   2. Halogens tend to be terminal
4. Place a pair of e- or a "–" between the central atom and all other atoms obeying the OCTET rules (some exceptions: H(2), Be(4), B(6))
5. Distribute ALL remaining pairs of e- on the terminal atoms to fill to an octet (H is a duet – 2).
   1. If any pairs of e- remain, then place them on the central atom.
   2. If after all pairs are placed and the octet rule is not satisfied, then make double or triple bonds

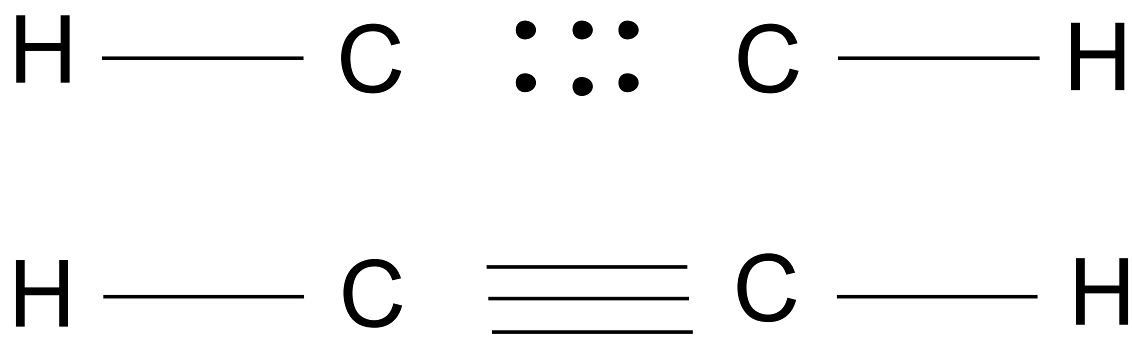
Multiple Covalent Bonds:
Double bonds



Ethene

Two pairs of shared electrons

Multiple Covalent Bonds:
Triple bonds



Ethyne

Three pairs of shared electrons