Agenda

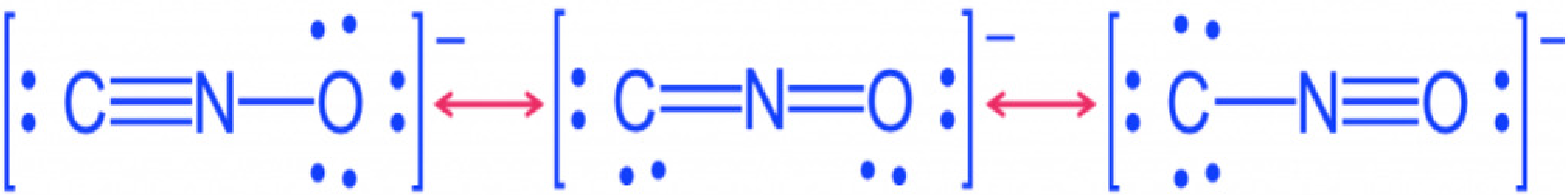
- Goals bellwork
- 2.6 Notes
- 2.6 Practice Problems
- 2.7 lab
  - Virtual on pHet simulation
  - Make 3D models
- 2.7 notes
- 2.7 practice problems

TOPIC 2.6: FORMAL CHARGE & RESONANCE

Enduring Understanding	
SAP-4	Molecular compounds are arranged based on Lewis diagrams and Valence Shell Electron Pair Repulsion (VSEPR) theory.
Learning Objective	
SAP-4B	Represent a molecule with a Lewis diagram that accounts for resonance between equivalent structures or that uses formal charge to select between

Formal Charge

When drawing Lewis Dot diagrams for some molecules and polyatomic ions, there can be several structures drawn.



Formal Charge is a method that can help determine which structure is most valid.

Calculating Formal Charge

TO CALCULATE THE FORMAL CHARGE FOR EACH ATOM IN THE MOLECULE:

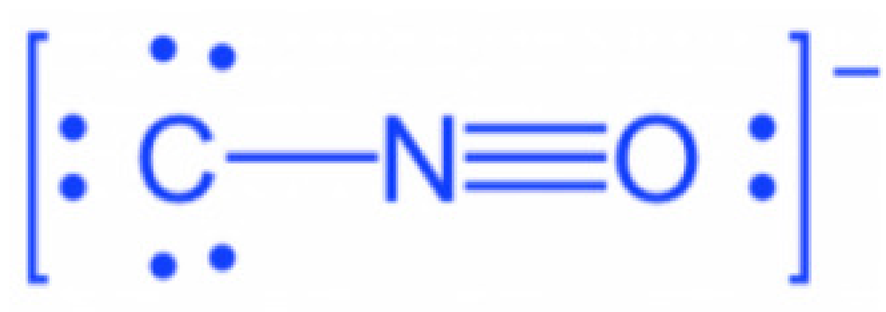
1. Determine the number of valence electrons of the atom.

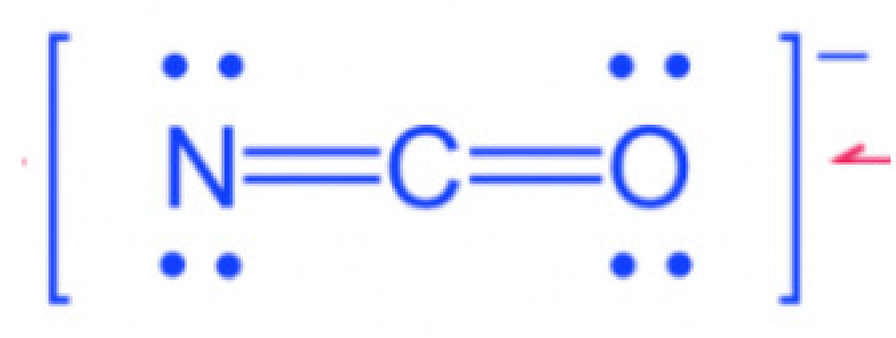
2. Subtract the sum of the lone electrons and bonds connected to the atom from the valence electrons.

*CHECK YOUR FORMAL CHARGE CALCULATION:

- The sum of the formal charges of each atom should add up to zero for a molecule or add up to the charge for a polyatomic ion.

Example: Two Resonance Structures of the Cyanate Ion



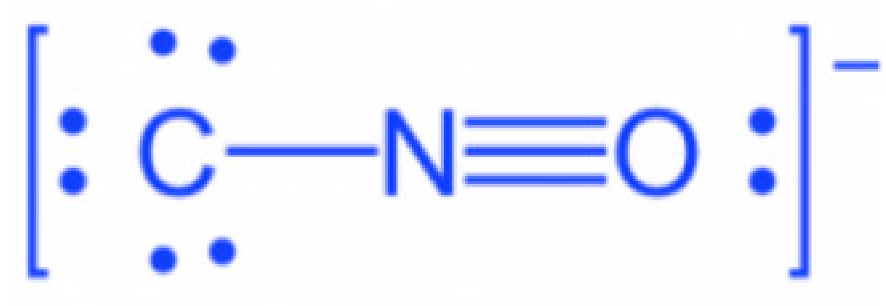


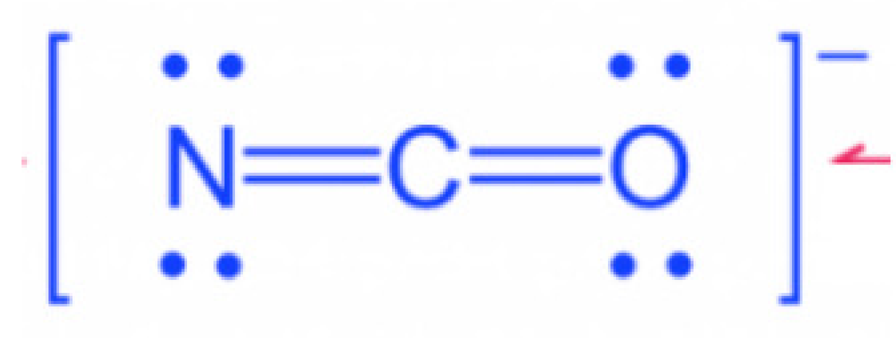
Valid Structures

The most valid structure will have:

- Formal Charges as close to zero for all atoms. (Most preferable is "no formal charge.")
- Negative Formal Charges will be placed on the most electronegative atom.

Which Resonance structure of cyanate is more valid?

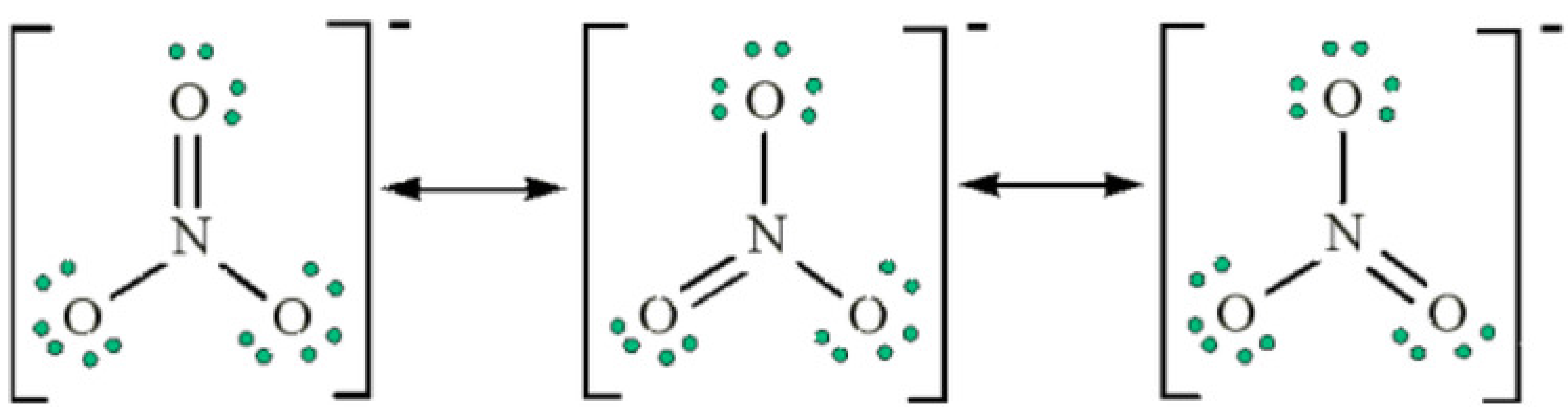




Draw an even more valid structure of cyanate:

Resonance Structures

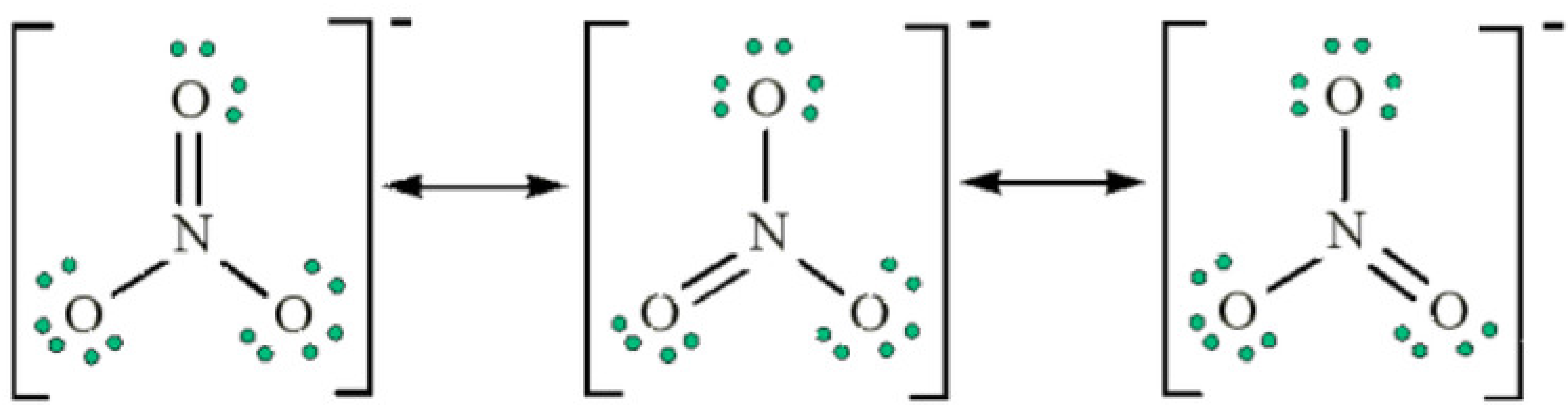
Sometimes when drawing a Lewis Structure you might find that there is more than one arrangement of bond/electrons that are equally valid.



Resonance Structures

Draw all the structures of the molecule, keeping the arrangement of the atoms the same but changing the location of the electrons.

Double arrows are drawn between the structures indicating that the actual structure is an average of the resonance structures.



Resonance Structures

Resonance structures are present simultaneously; they do not flip between them.

The electrons can be described as delocalized. Charge is shared.

Bond lengths are an average of the bonds present. In the NO_2^{1-} ion the bond length is between a single and double bond.

Together

1. Calculate the formal charges for each atom in the molecule in hydrogen cyanide, HCN.

2. Draw the resonance structures of the carbonate ion, CO_3^{2-}.

You do, we review

3. Calculate the formal charge of each atom in the sulfate ion, SO_4^{2-}.

4. Draw all resonance structures of SO_2.

TOPIC 2.7: VSEPR THEORY & BOND HYBRIDIZATION

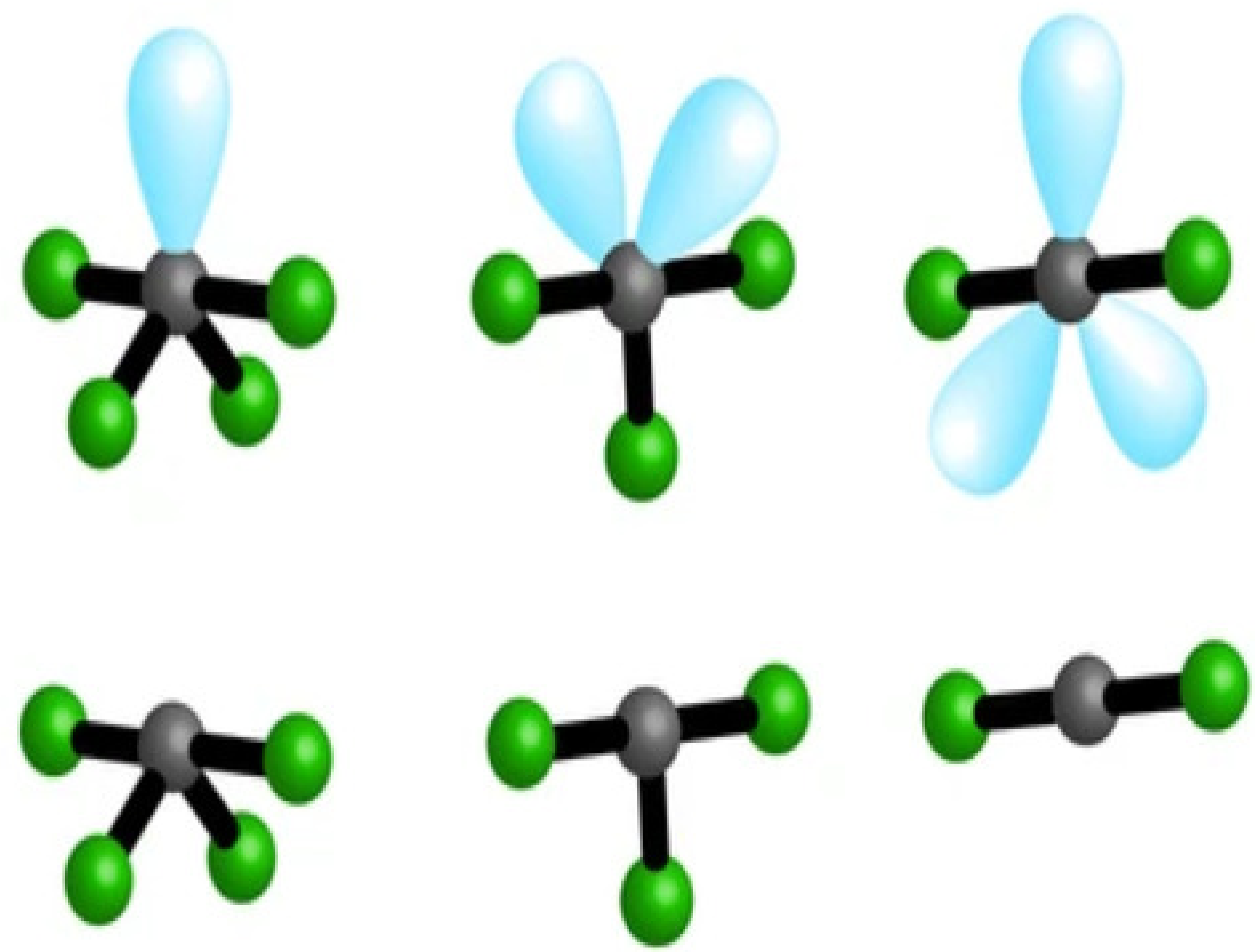
Enduring Understanding	
SAP-4	Molecular compounds are arranged based on Lewis diagrams and Valence Shell Electron Pair Repulsion (VSEPR) theory.
Learning Objective	
SAP-4C	Based on the relationship between Lewis diagrams, VSEPR theory, bond orders, and bond polarities: a. Explain structural properties of molecules. b. Explain electron properties of

VSEPR Lab

- Go to https://phet.colorado.edu/sims/html/molecule-shapes/latest/molecule-shapes_all.html and complete the virtual lab
- Then show Ms. Fortin and make 3D models using clay

VSEPR Theory

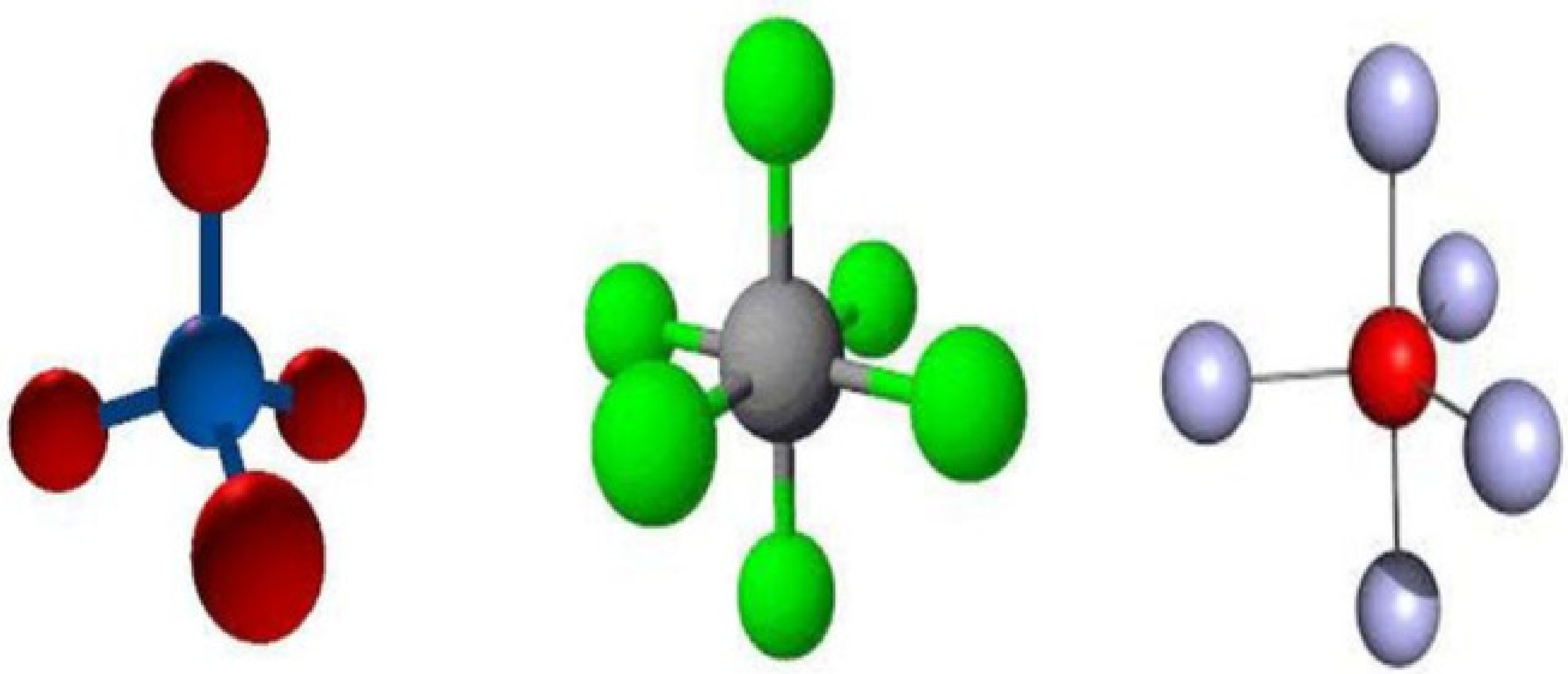
The valence shell electron-pair repulsion (VSPER) theory predicts the geometries of molecules and polyatomic ions.



VSEPR

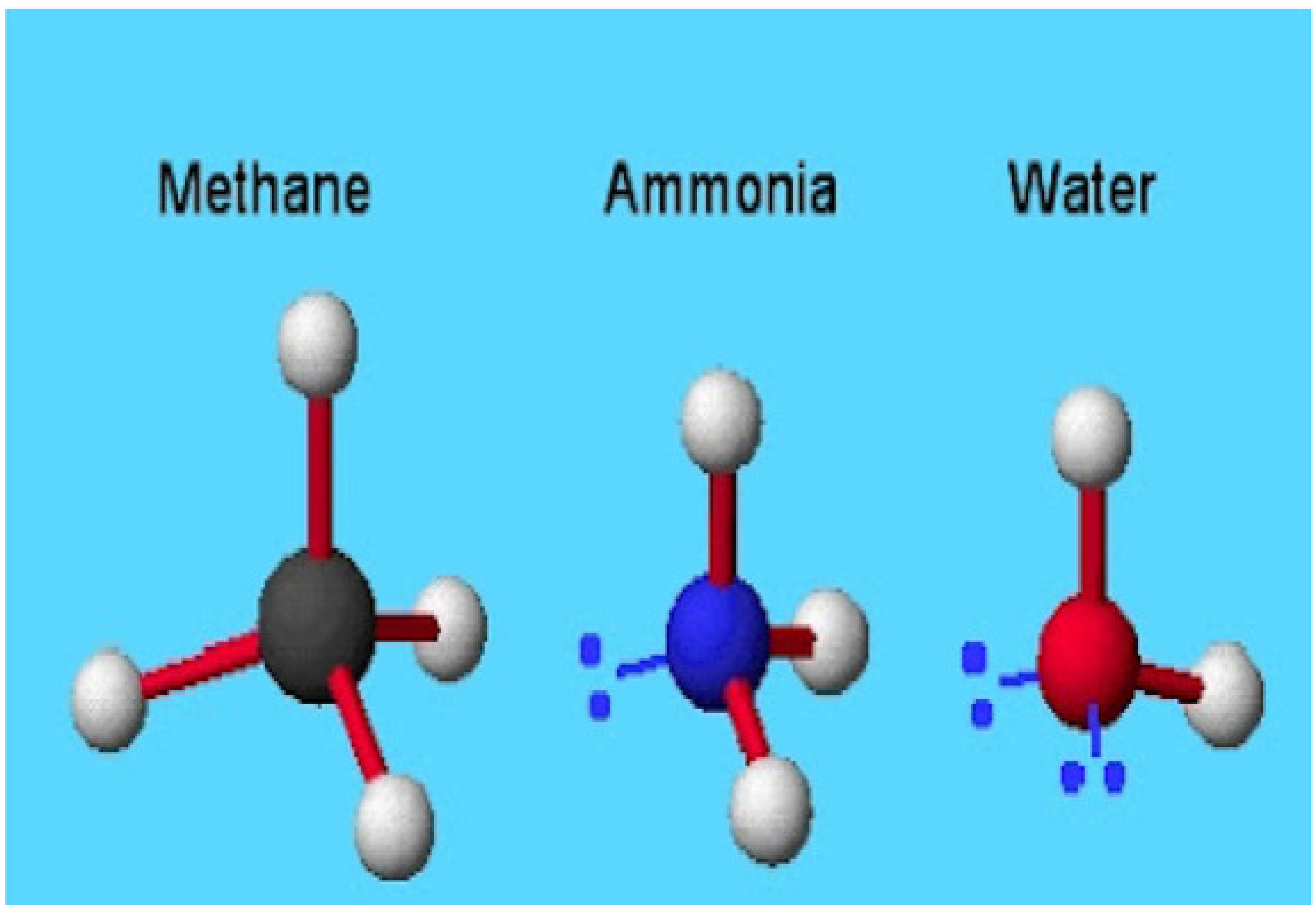
The shape, or geometry, of a molecule is determined by lone pairs or bonds on the central atom of a molecule.

Electron – electron repulsions are minimized by positioning themselves as far apart as possible.



Lone Pairs Vs. Bonding Pairs

Lone pairs of electrons repel more than bonds and tend to compress the angle between bonding atoms.



Determining Molecular Geometry

1. Draw the Lewis structure of the molecule.
2. Count the electron domains (bonds and lone pairs) around the central atom.
   a. For structures with double or triple bonds, count the multiple bond(s) as one
   b. If there is a single electron (as in an odd electron molecule such as NO_3), count the odd electron as its own lone pair.
3. Use the arrangement of the lone pairs and bonds to determine the molecular geometry. *You must memorize these geometries and bond angles for the AP Chem exam.
4. If there is more than one central atom we determine the geometric shape of each central atom individually by following the same steps above for each central atom.

Bond Hybridization

- What is the electron configuration for C?
- This implies that C can form how many bonds?
- How many bonds can carbon actually form?

Bond Hybridization

- Atomic orbitals on an atom mix to form hybrid orbitals.
- The shape of a hybrid orbital is a mix of the shapes of the original atomic orbitals such as s and p
- The total number of atomic orbitals on an atom remains constant, so the number of hybrid orbitals on an atom equals the number of atomic orbitals that are mixed.
- In methane, (CH_4), the 2s and three 2p orbitals of carbon mix to form four sp^3 hybrid orbitals.

Bond Hybridization

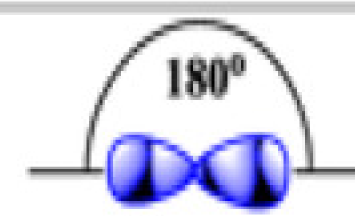
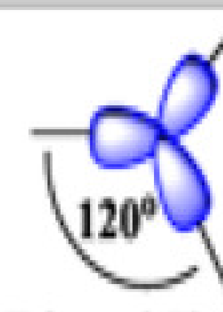
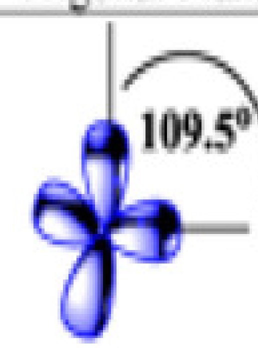
The sum of the superscripts on the hybrid orbitals equals the number of electron clouds around the central atom.

The carbon atom in CH_4 has 4 electron clouds around it.

The sum of the superscripts in sp^3 equals 4.

You will need to identify sp, sp^2 and sp^3 hybridization in AP Chemistry.

Hybrid Orbitals and Geometry

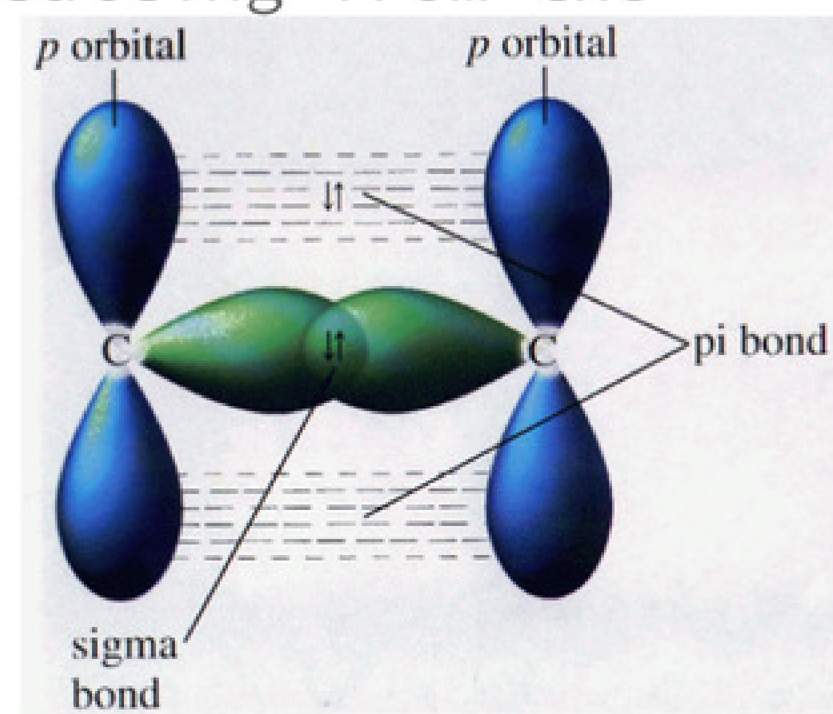
Atomic Orbitals Used	Hybrid Orbitals Formed	Geometry	Example Compound
s,p	Two sp orbitals	 Linear	CO_2
s,p,p	Three sp^2 orbitals	 Trigonal Planar	SO_3
s,p,p,p	Four sp^3 orbitals	 Tetrahedral	$GeCl_4$

Sigma & Pi Bonds

Sigma bonds (σ) are always the first bond between two atoms - a single bond.

Pi bonds (π) are second and third bonds resulting from the overlap of p orbitals.

Single bond	1 sigma bond
Double Bond	1 sigma, 1 pi bond
Triple Bond	1 sigma, 2 pi bonds



Bond Length, Strength, & Energy

As the number of bonds between two atoms increases:

- Bond strength increases
- Bond energy increases
- Bond length decreases

Pi bonds pull the atoms closer together.

- Triple bonds are the strongest and shortest bonds with the highest energy
- Single bonds are the longest and weakest bonds with the lowest energy.

Bond Order

Bond order is the number of bonding pairs of electrons between two atoms

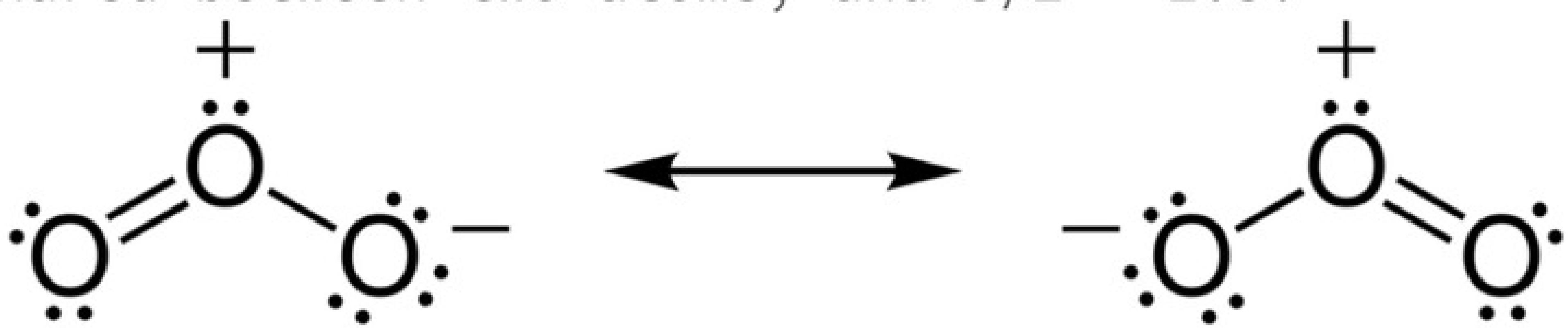
Bond Type	Bond order
single	1
double	2
triple	3

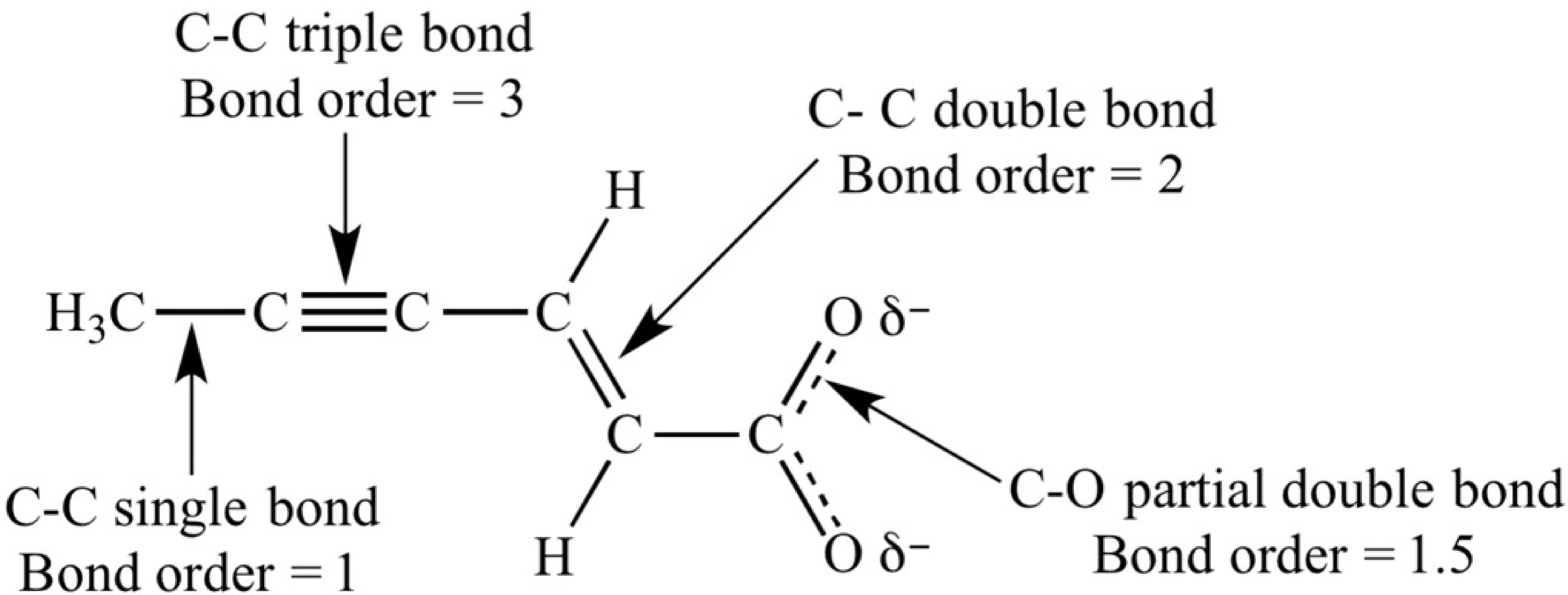
Bond order and Resonance

For a molecule that exhibits resonance, bonds that have resonance are experimentally determined to be the same length.

In ozone, O_3, both bonds have a bond length that is halfway between a single and double bond, so the bond order is halfway between a single and double bond order, and it’s bond order is 1.5.

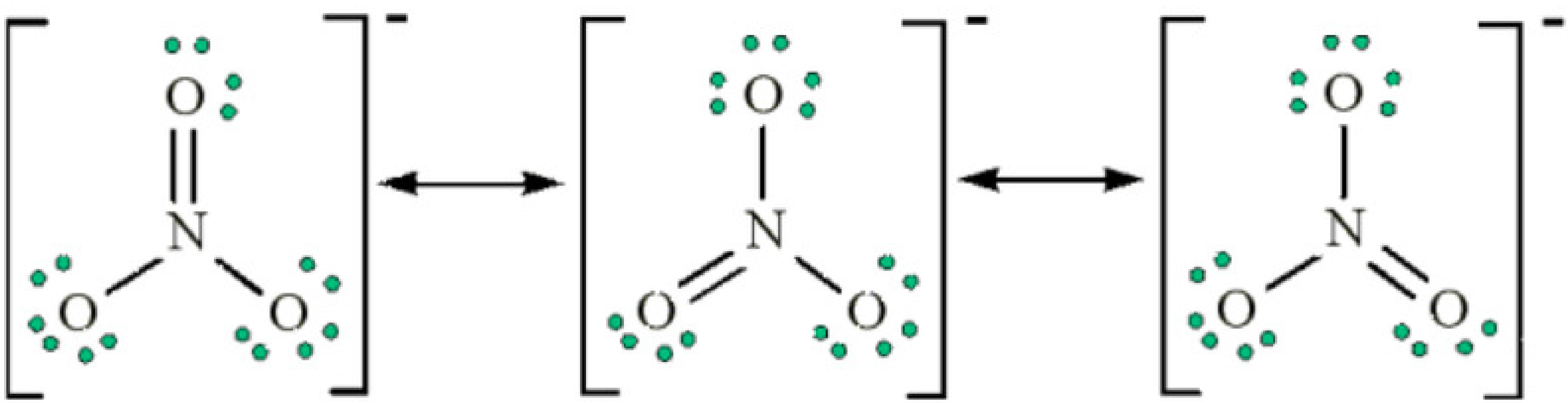
Another way to think about this is that there are three bonds shared between two atoms, and 3/2 = 1.5.




C-C triple bond
Bond order = 3
C- C double bond
Bond order = 2
H
H_3C
C
C
C
O δ⁻
C
C
C-O partial double bond
Bond order = 1.5
C-C single bond
Bond order = 1
H
O δ⁻

Bond Order and Resonance

In the nitrate ion, NO_3^-, there are four bonds shared by the nitrogen with each of the three oxygen atoms. The bond order is 4/3 = 1.33

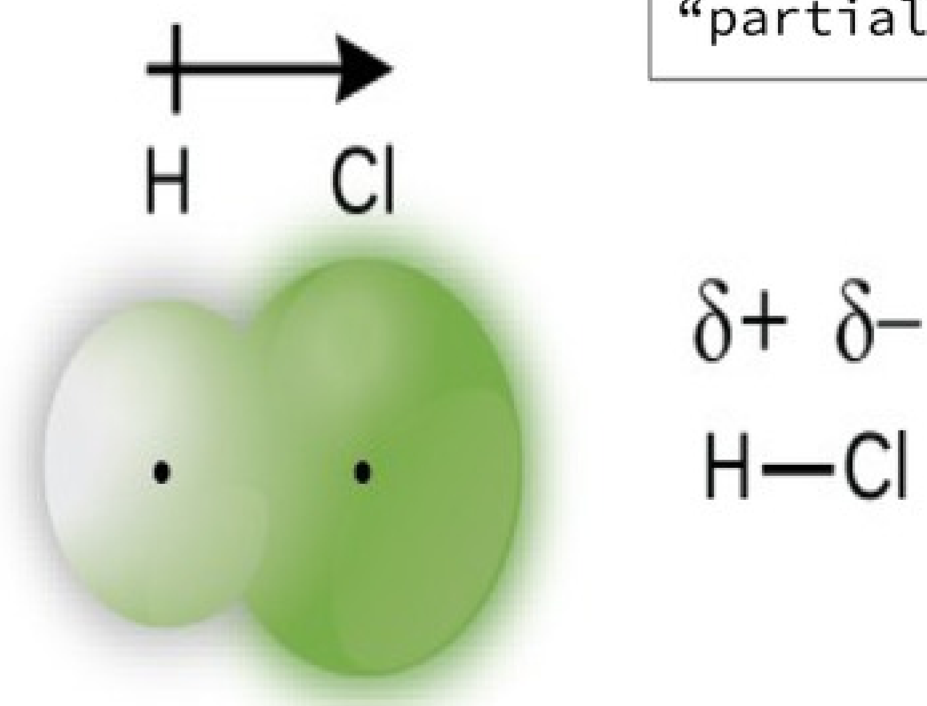


Bond Polarity

When electrons are shared in a covalent bond, the shared electrons spend more time around the more electronegative element in the bond.

This gives the more electronegative element a slightly negative charge (□-) and the less electronegative element a slightly positive charge (□+) resulting in a polar molecule.

*Arrow always points toward the more electronegative atom.



*δ means "slightly" or "partial"

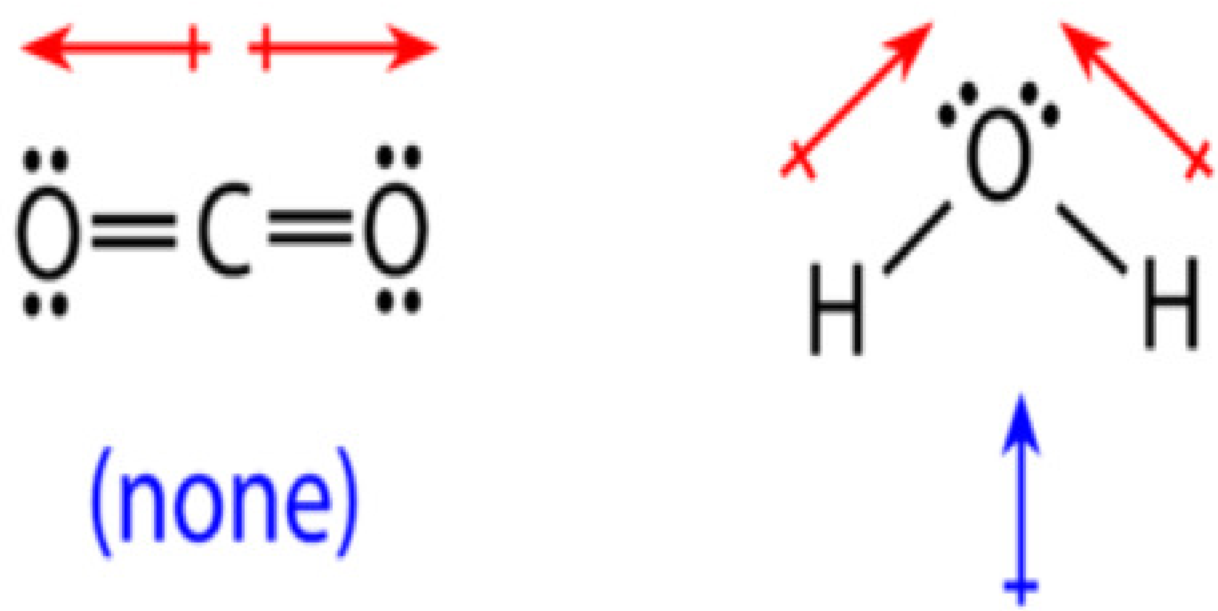
*HCl is a polar molecule because there is a **dipole** moment that isn't canceled out.

Molecular Polarity

If a molecule is polar, it has a dipole moment. To know if a molecule is polar, you need to know if the bonds are polar (have a difference in electronegativity) and the overall shape of the molecule.

Bond Dipoles:

Molecular Dipoles:



Together

1. Determine the molecular geometry and predict the bond angles of the following:
    a. ICl_2^-
    b. SOF_4

Together

2. Draw a Lewis structure for the following chemical species. Indicate the hybridization on the central atom and the total number of sigma and pi bonds in the molecule.

   a. CN^-

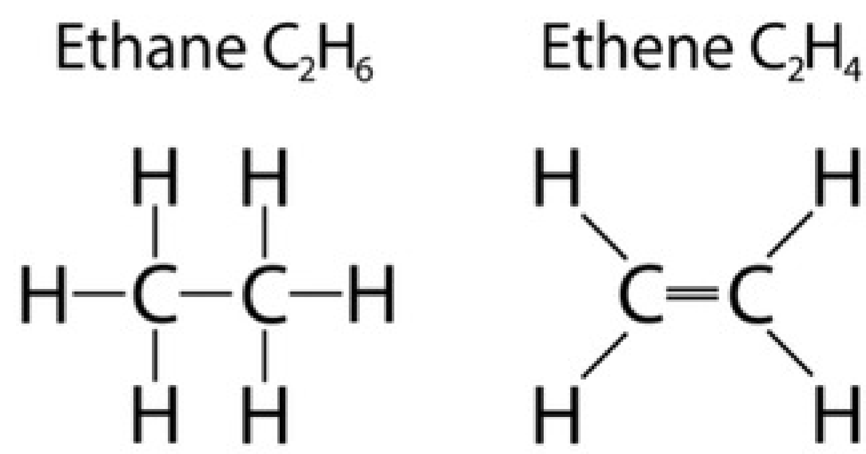
   b. H_2CO

Together

3. Is ammonia, NH_3, polar or nonpolar? Explain using molecular shape, polar bonds, and indicate if there is a molecular dipole using an arrow.

TOGETHER

4. Consider the Lewis structures for ethane and ethene.
   a. The carbon-carbon bond in which molecule has the highest bond order?
   b. The carbon-carbon bond in which molecule has the lowest bond energy?



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5. Draw the Lewis structures for ethyne, C_2H_2 and carbon dioxide, CO_2. Predict the molecular geometries and the bond angles for each molecule.

6. When the following reaction occurs, does the hybridization of the carbon atoms change? Explain.

$$2C_2H_2 + 5O_2 \rightarrow 4CO_2 + 2H_2O$$

You Do We Review

In the Lewis structure below determine:

a. the hybridization of each carbon atom labeled 1, 2, 3, 4 and 5
b. the bond angles of A1, A2 and A3
c. the total number of sigma and pi bonds in the molecule