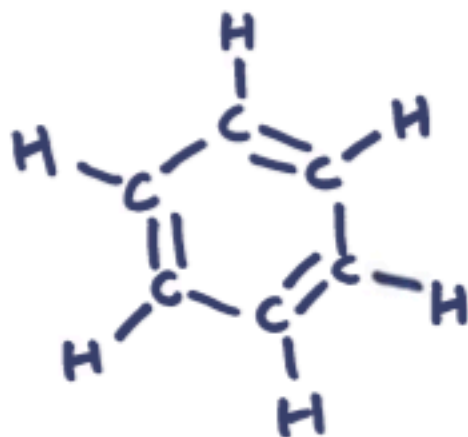
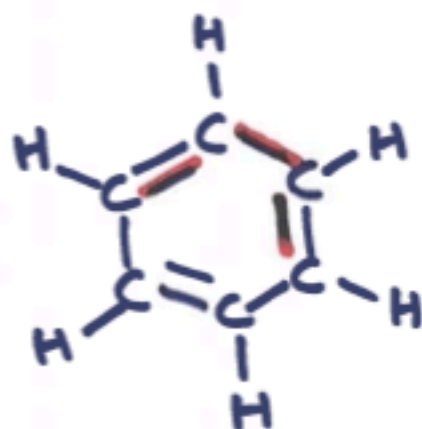


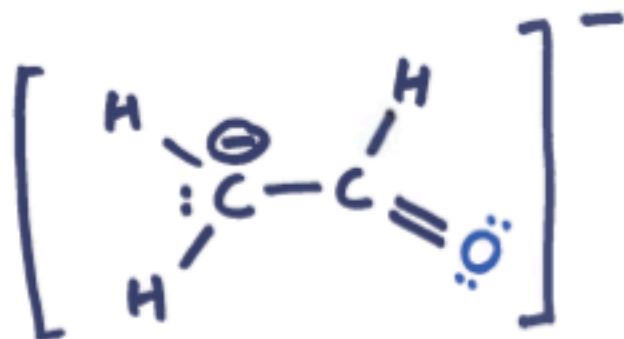
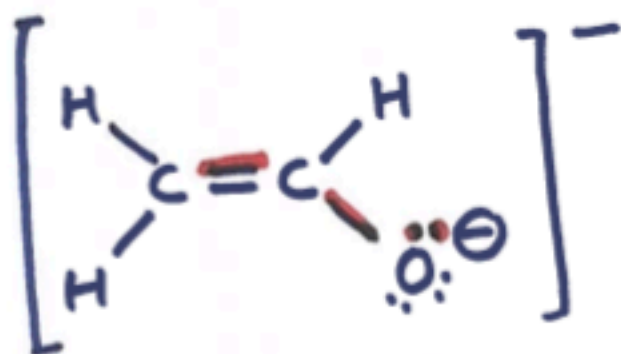
Resonance Patterns

(Sep. 20th/2023)

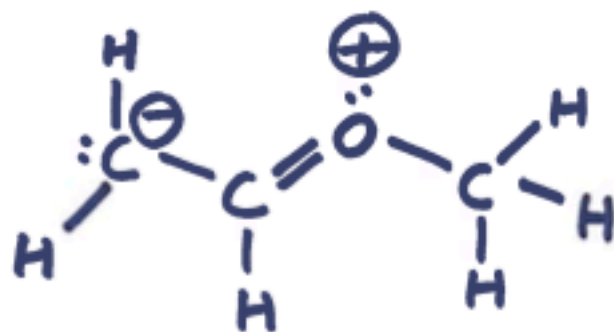
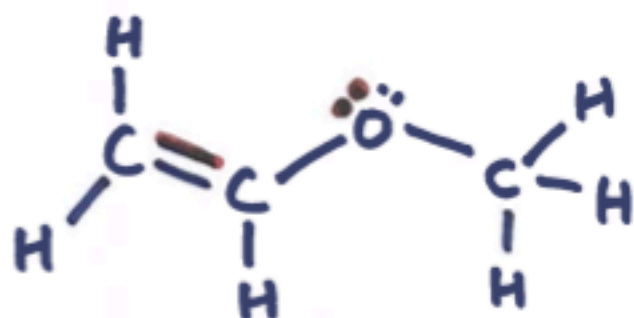
① $\pi - \sigma - \pi$



② $\pi - \sigma - \text{charge}$



③ $\pi - \sigma - \text{lone pair}$





Welcome to Chemistry 154!

Please make sure to sync your iClicker Cloud
to Chem154 Section 113

Based on this cat scale....how do you feel today?





Reminders

- **Worksheet: Unit 3 (Qs 1-10)**
- Due September 26th at 11:59pm
- **Worksheet: Unit 3 (Questions 16-22)**
- Due Oct. 2nd at 11:59pm
- **Achieve Assignment #3**
- Due Oct. 2nd at 11:59pm

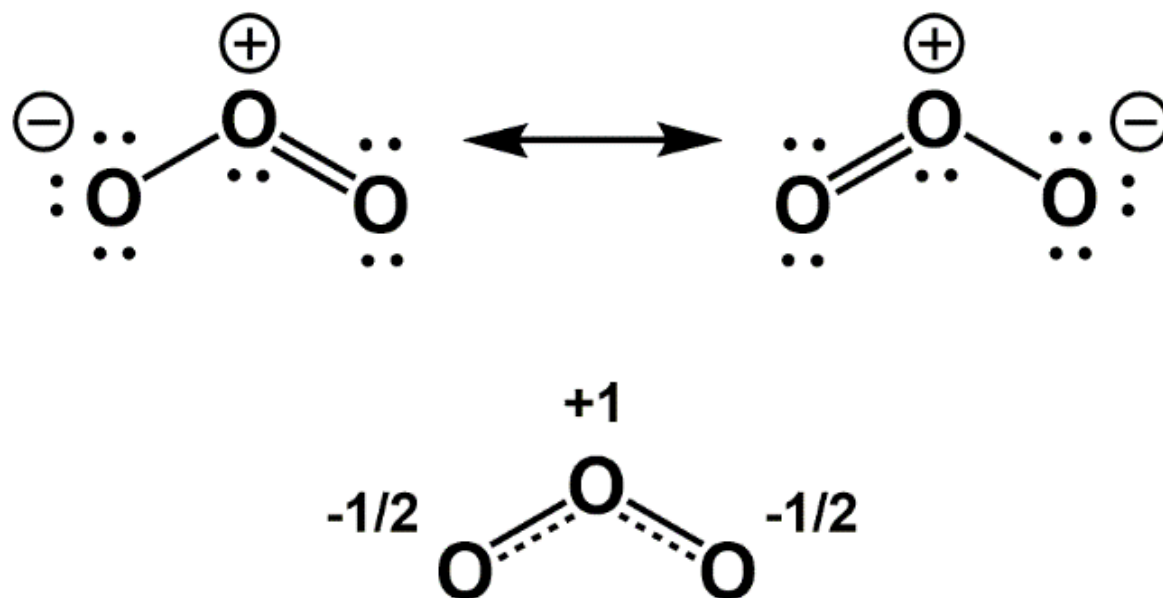
Instructor Office Hours

Monday and Friday 7-8pm via Zoom (All Lectures Site)

Resonance structures

Resonance occurs when **the same arrangement of atoms** produces more than one Lewis structure. This indicates a delocalized bond (extending beyond two atoms) is present. These structures contribute to the resonance hybrid (the actual molecular structure).

Resonance Hybrid is a
“true” bonding picture.
It is NOT a Lewis
structure.

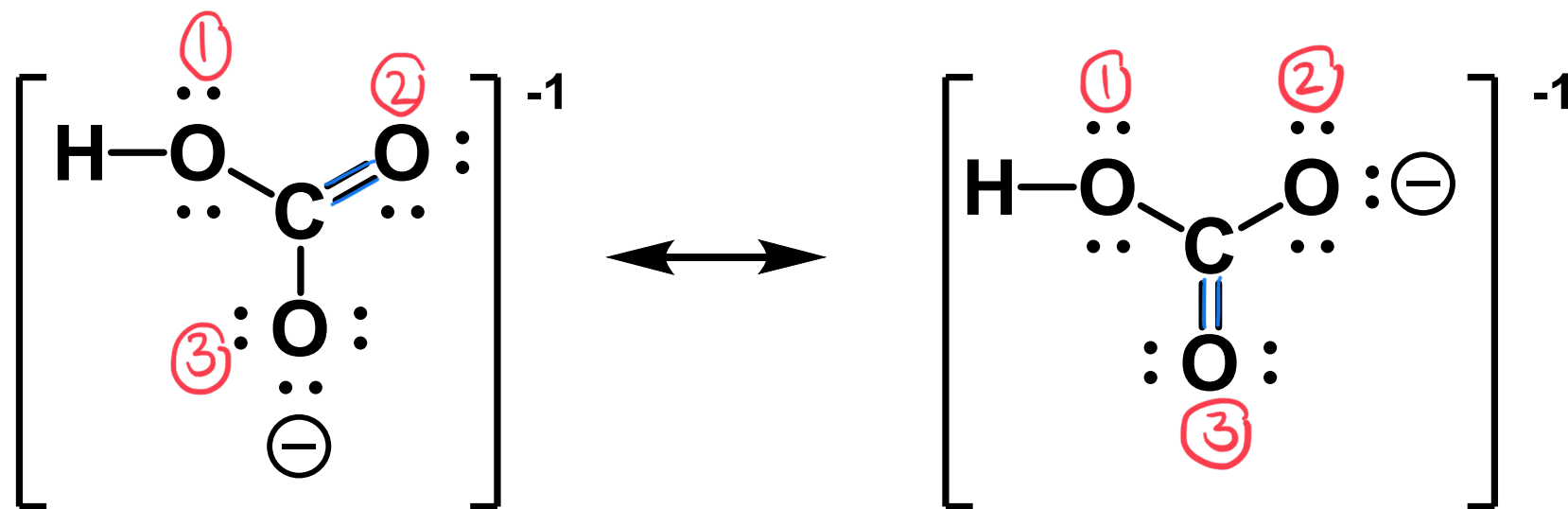


Drawing Resonance Structures

- Only **electrons** can be moved – nuclei NEVER move in resonance structures
- Total number of electrons in system is constant, total charge in system is constant
- All structures should be proper Lewis structures
- *Look for lone pair and double-bond electrons. These move in resonance structures.*

Clicker Question

True or False: Are the following structures contributing to the same resonance hybrid of the $[\text{HCO}_3]^-$ anion?

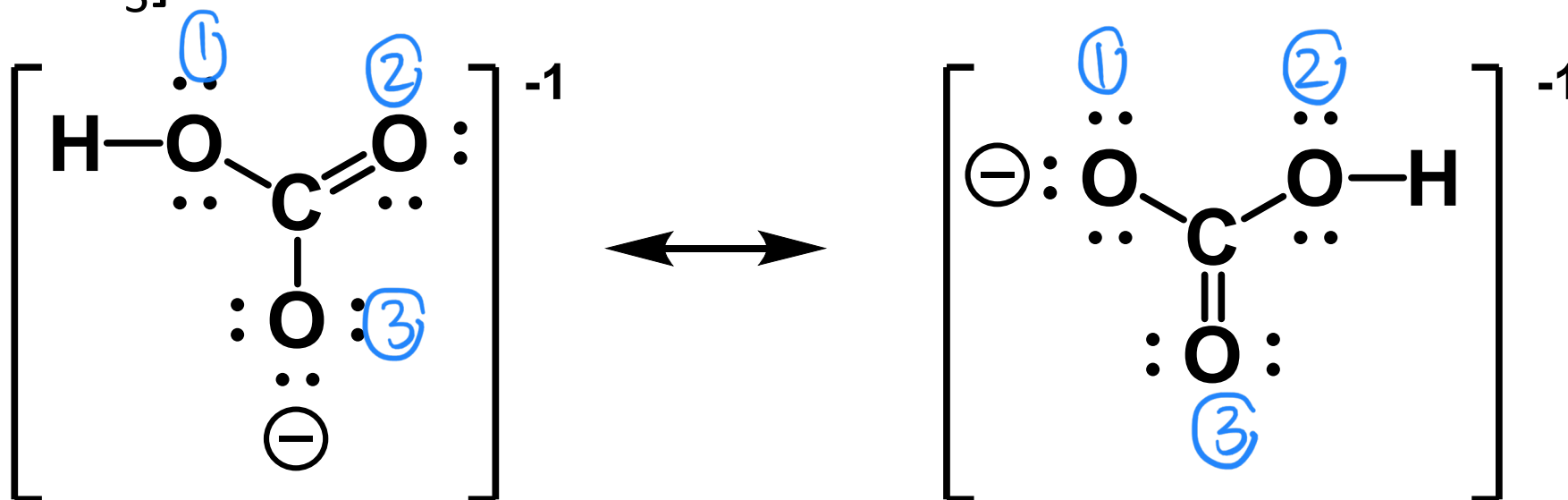


a. True

b. False

Clicker Question

True or False: Are the following structures contributing to the same resonance hybrid of the $[\text{HCO}_3]^-$ anion?

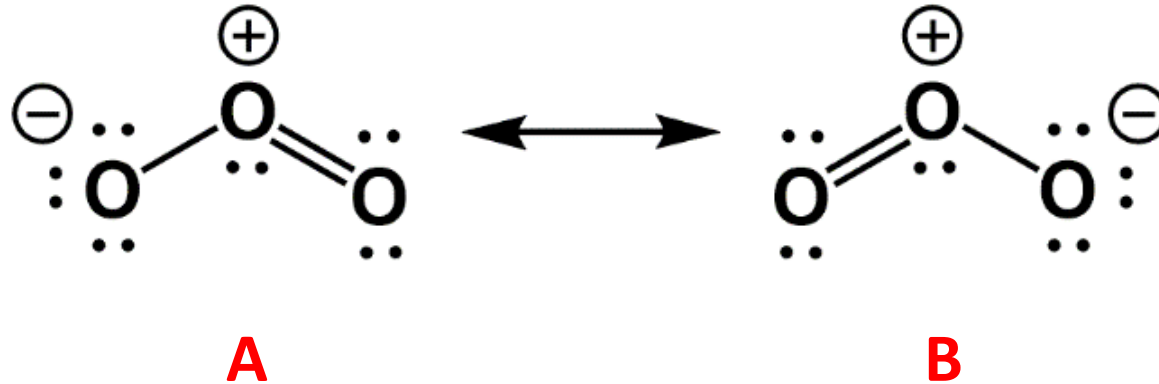


a. True

b. False

Atoms do NOT move between resonance structures. Only the electrons!

Clicker Question



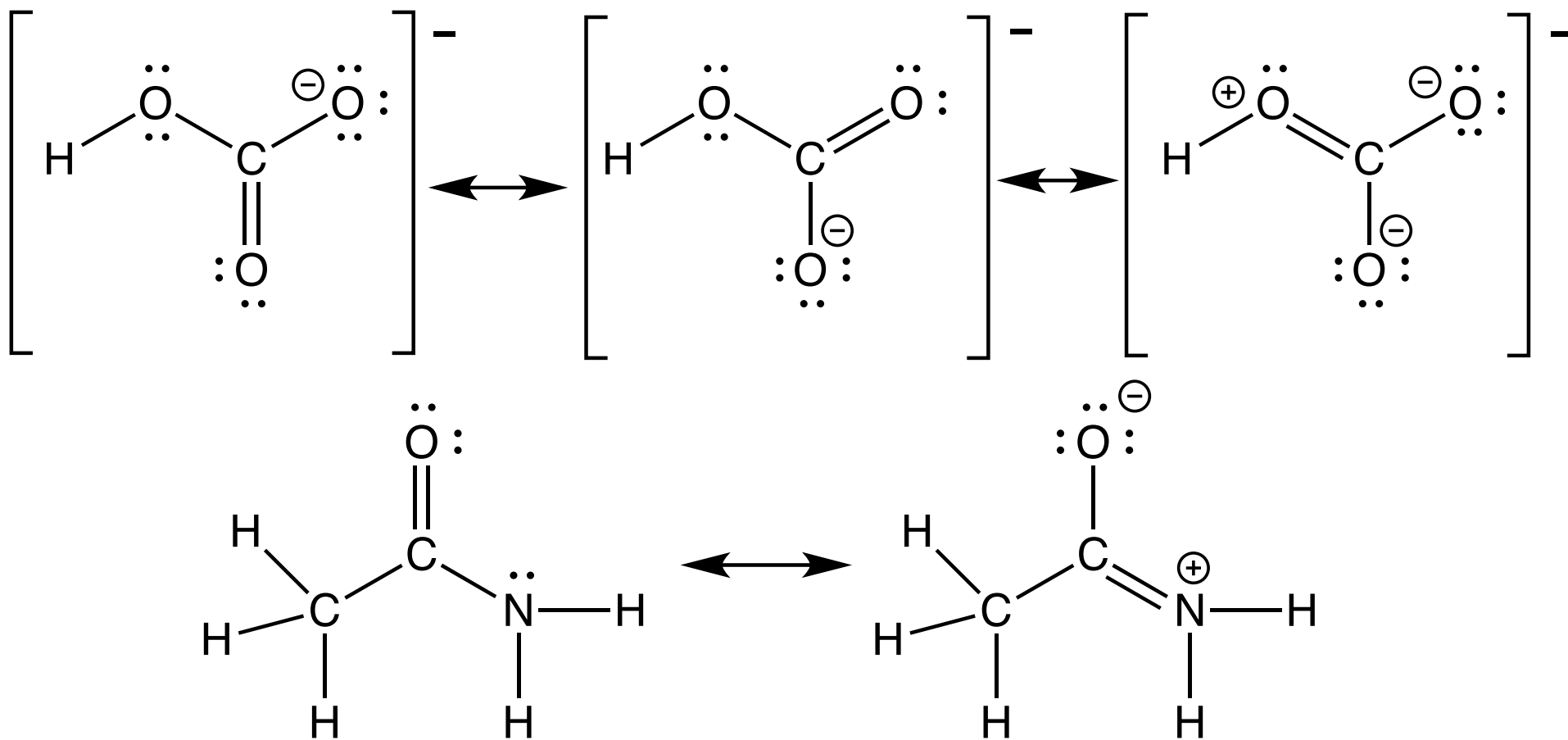
An engineer is able to characterize a 1 M solution of ozone by observing the O-O bonds in the molecule. What will they observe?

- a) An equal mixture (1:1) of molecules A and B
- b) An equilibrium mixture of molecules A and B
- c) Molecules quickly converting between A and B
- ☒ d) None of molecules A or B will be observed

Stability of Resonance Contributors

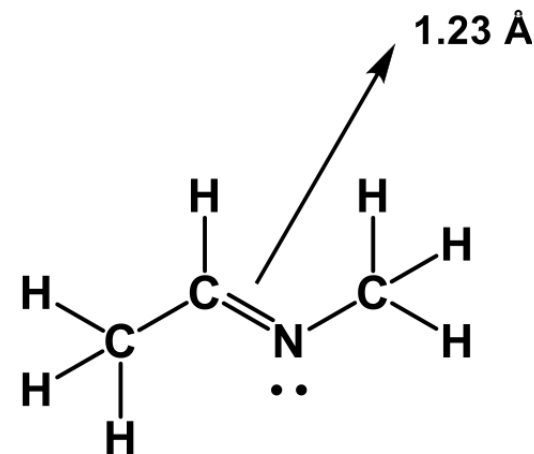
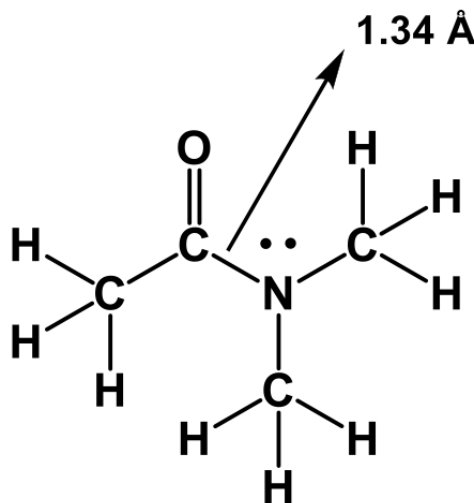
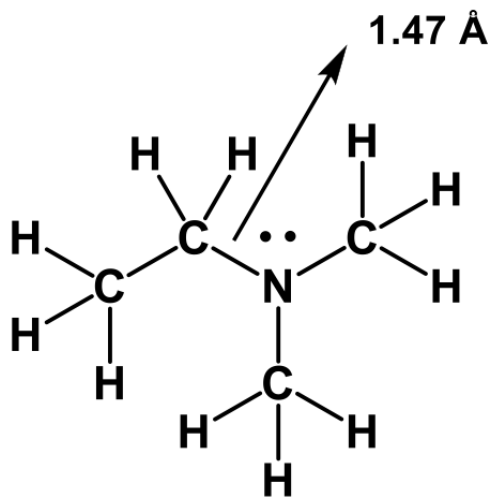
Resonance contributors may not all have the same stability.

Better (more stable) Lewis structures will make a stronger contribution to structure of the resonance hybrid.



Worksheet Question #14 – GOOD QUESTION

The carbon-nitrogen bond length for three organic compounds is shown below. Briefly explain this trend.



Worksheet Question #12

Draw ALL chemically reasonable Lewis structures (including resonance structures) of SO_2F_2 having S as the central atom. Propose reasons why the linearly-connected structure F-O-S-O-F is not found in nature.

Click any answer on your clicker when you have finished this worksheet question!

Worksheet Question #12 (Clicker)

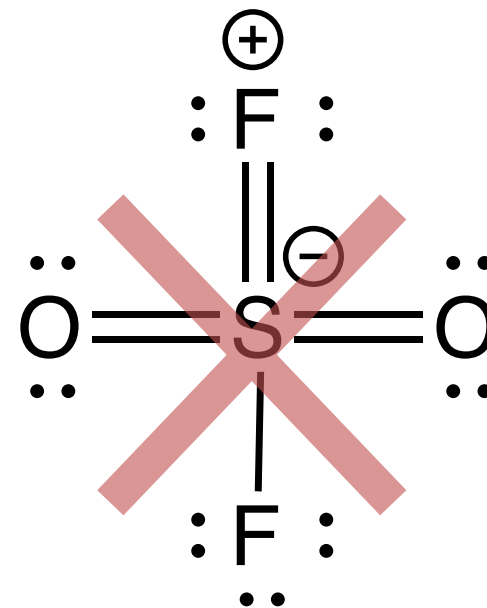
How many chemically reasonable resonance structures does SO_2F_2 have?

- a) 1
- b) 2
- c) 3
- ☒ d) 4
- e) More than 4

Worksheet Question #12 (Clicker)

What is wrong with the Lewis structure of SO_2F_2 shown?

- A) The positive formal charge is on the electronegative fluorine atom
- B) Fluorine is hypervalent
- C) The negative formal charge is on the (less) electronegative sulfur atom
- D) Answers A + B
- E) Answers A + C



Hypervalency and resonance

In CHEM 154, if multiple **hypervalent** resonance structures are possible, only those having positive or zero formal charges on the central atom are considered valid.

Do NOT put a negative formal charge on the central atom unless you absolutely have to (i.e. there are no better resonance structures).

In CHEM 154, you should NEVER put a double bond on a halogen (group 17).

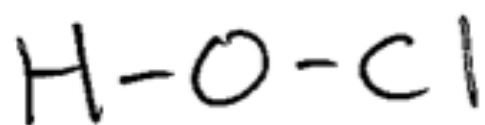
Worksheet Question #3

Hypochlorous acid has the molecular formula HOCl. There are four possible ways to arrange the atoms in HOCl. Draw four possible **skeletal** structures showing atom connectivity below:
(you do not need to draw full Lewis structures).

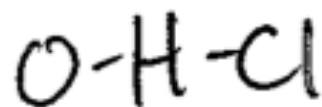
For each of the structures above, briefly explain why it can or cannot be a valid Lewis structure for HOCl

Worksheet Question #3 – Clicker

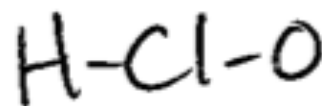
The best **Lewis structure** for HOCl is based on which of the following skeletal connectivities:



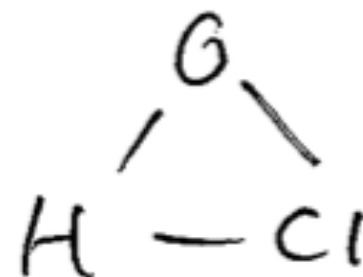
A



B



C



D

Learning Objectives (Part 2)

After mastering this unit you will be able to:

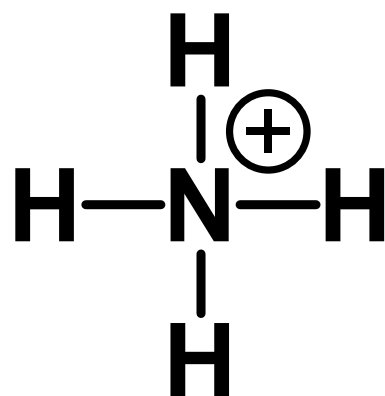
- Predict the geometry (shape, approximate bond angles, and trends in bond lengths) of molecules from their Lewis structures.
- Predict the polarity of a molecule from its molecular geometry and bond polarity.

Shapes of Molecules

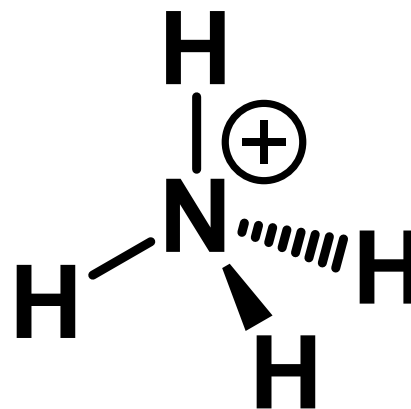
Lewis structures provide information about molecular bonding but they do NOT provide any information on molecular geometry. Molecular geometry is important in determining a substance's properties such as reactivity, solubility, and even conductivity in solids.

Valence Shell Electron Pair Repulsion (VSEPR)

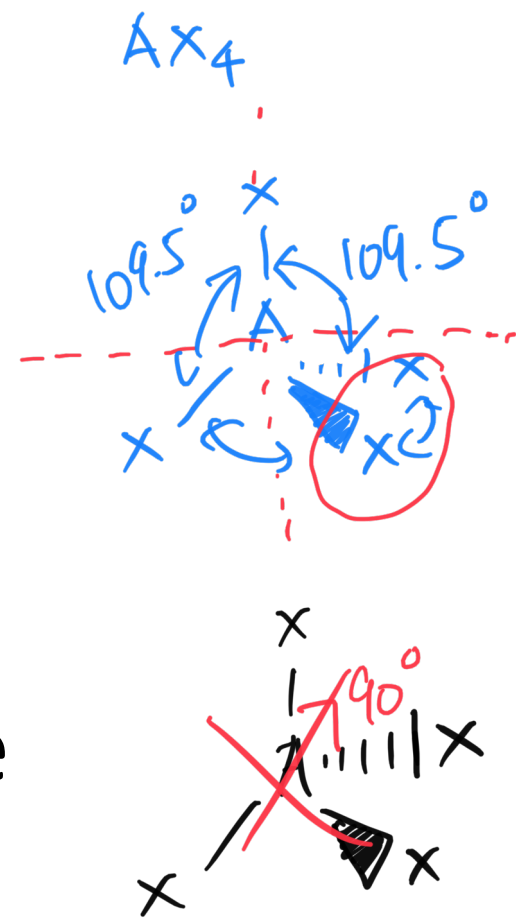
VSEPR is a theory that predicts molecular shape by treating atoms in a molecule as point charges that are favoured to be as far away from each other as possible.





Lewis
structure



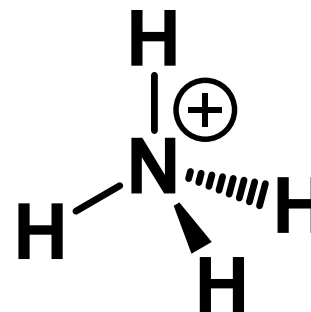
Perspective
diagram



Perspective Diagram

A perspective diagram is a three-dimensional representation of a molecule in space. A wedge bond () represents an atom coming out of the plane of the molecule. A dash bond () represents an atom going into the plane of the molecule.

Perspective Diagram



Note: for this tetrahedral shape, the dash and wedge bonds should both lie **below** a horizontal line drawn through the central atom.

VSEPR Guidelines

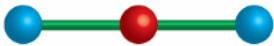
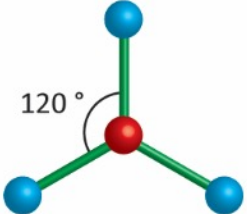
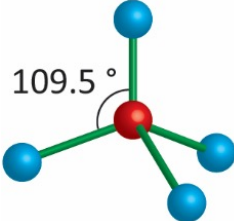
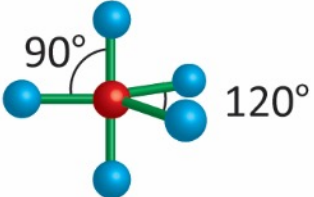
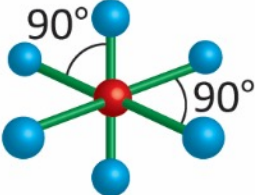
- You do NOT need to show lone pairs in VSEPR perspective diagrams
- You do NOT need to draw multiple bonds in VSEPR perspective diagrams

Predicting Molecular Geometry

1. Draw the best Lewis structure
2. Determine the parent shape (lone pairs + number of atoms directly bonded to the central atom)
3. Determine the molecular shape

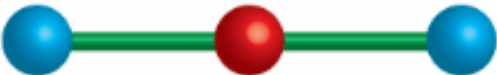
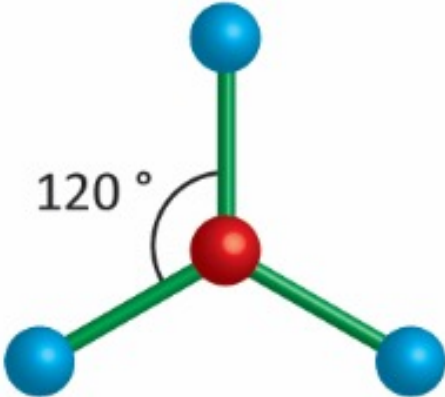
Parent Shapes

The five parent shapes describe how atoms and/or lone pairs arrange in a molecule to reduce electrostatic interactions.

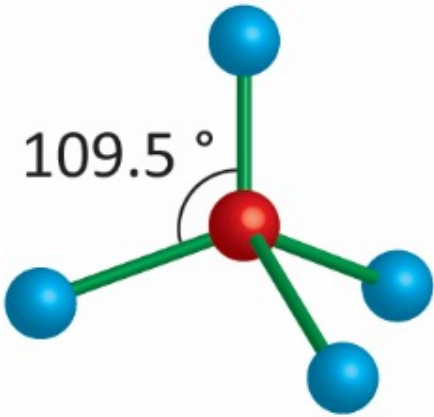
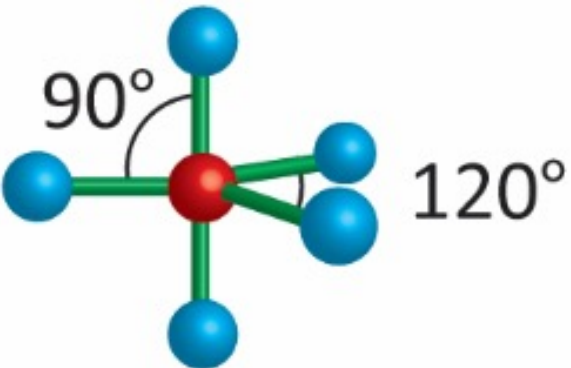
# of bond pairs or lone pairs around the central atom	Parent shape	Bond angles	Structure (blue spheres represent atoms or lone pairs)
2	Linear	180°	 A central red sphere is bonded to two blue spheres in a straight line, representing a linear geometry with a bond angle of 180 degrees.
3	Trigonal planar	120°	 A central red sphere is bonded to three blue spheres in a flat triangle, representing a trigonal planar geometry with bond angles of 120 degrees.
4	Tetrahedral	109.5°	 A central red sphere is bonded to four blue spheres in a tetrahedral arrangement, representing a tetrahedral geometry with bond angles of 109.5 degrees.
5	Trigonal bipyramidal	$120^\circ / 90^\circ$	 A central red sphere is bonded to five blue spheres in a trigonal bipyramidal arrangement. The equatorial bond angles are 120 degrees, and the axial bond angles are 90 degrees.
6	Octahedral	90°	 A central red sphere is bonded to six blue spheres in an octahedral arrangement. The bond angles between adjacent spheres are 90 degrees.

Parent Shapes

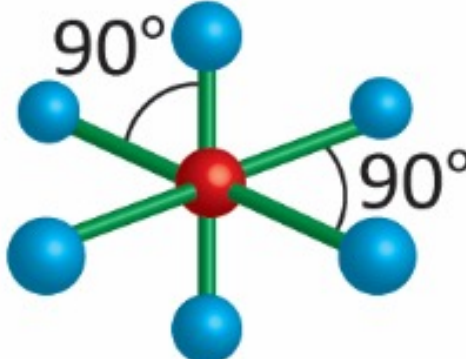
The five parent shapes describe how atoms and/or lone pairs arrange in a molecule to reduce electrostatic interactions.

# of bond pairs or lone pairs around the central atom	Parent shape	Bond angles	Structure (blue spheres represent atoms or lone pairs)
2	Linear	180°	 A diagram showing a linear arrangement of three spheres. A central red sphere is connected by green lines to two blue spheres on either side, forming a straight line.
3	Trigonal planar	120°	 A diagram showing a central red sphere connected by green lines to three blue spheres. The three blue spheres are arranged in a triangle around the central red sphere, with a curved arrow indicating a bond angle of 120° .

Parent Shapes

# of bond pairs or lone pairs around the central atom	Parent shape	Bond angles	Structure (blue spheres represent atoms or lone pairs)
4	Tetrahedral	109.5°	
5	Trigonal bipyramidal	$120^\circ / 180^\circ$	

Parent Shapes

# of bond pairs or lone pairs around the central atom	Parent shape	Bond angles	Structure (blue spheres represent atoms or lone pairs)
6	Octahedral	90°	

Molecular Shapes

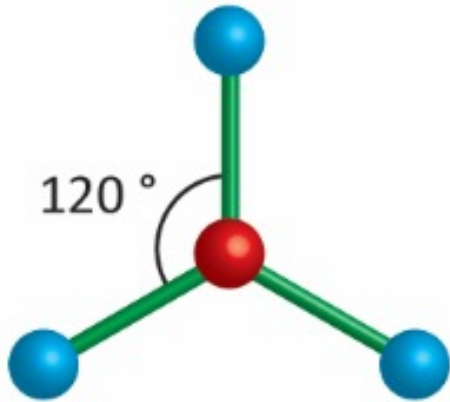
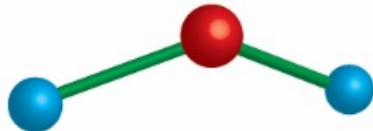
The molecular shape describes the three-dimensional arrangement of atoms in space to minimize electrostatic repulsions.

Note: LP – number of lone pairs

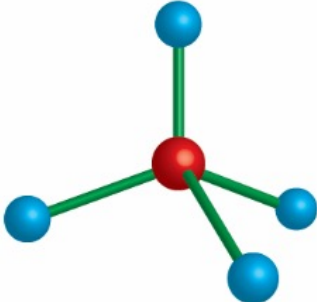
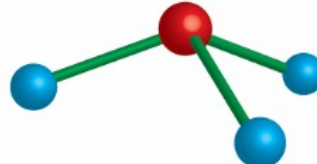
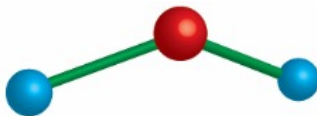
BP – number of bond pairs

- multiple bonds count as one here
- same as number of atoms bonded

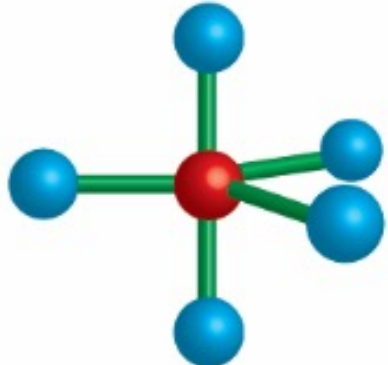
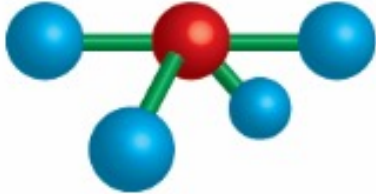
Trigonal Planar Parent Shape

Parent Shape	LP	BP	Molecular Shape	3D Structure
Trigonal Planar	0	3	Trigonal Planar	
Trigonal Planar	1	2	Bent	

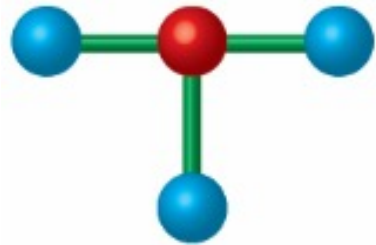
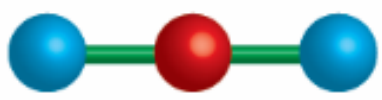
Tetrahedral Parent Shape

Parent Shape	LP	BP	Molecular Shape	3D Structure
Tetrahedral	0	4	Tetrahedral	
Tetrahedral	1	3	Trigonal pyramidal	
Tetrahedral	2	2	Bent	

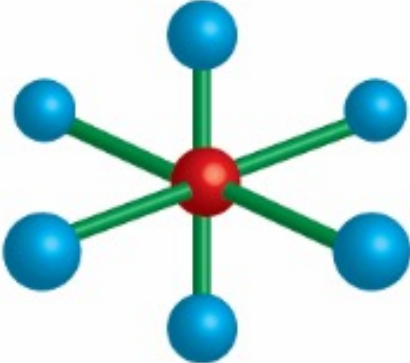
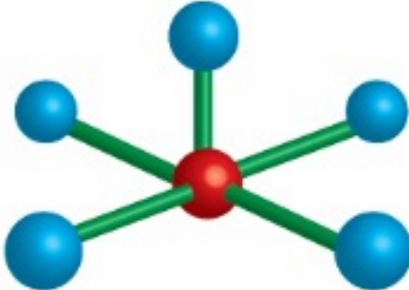
Trigonal Bipyramidal Parent Shape

Parent Shape	LP	BP	Molecular Shape	3D Structure
Trigonal Bipyramidal	0	5	Trigonal bipyramidal	
Trigonal Bipyramidal	1	4	See-saw	

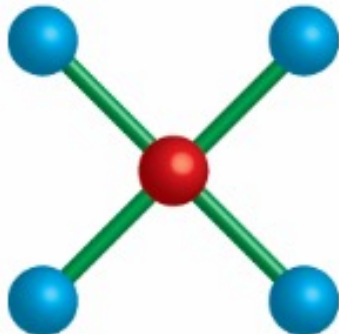
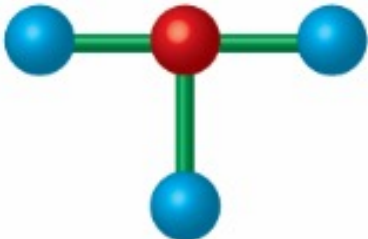
Trigonal Bipyramidal Parent Shape

Parent Shape	LP	BP	Molecular Shape	3D Structure
Trigonal Bipyramidal	2	3	T-shape	
Trigonal Bipyramidal	3	2	Linear	

Octahedral Parent Shape

Parent Shape	LP	BP	Molecular Shape	3D Structure
Octahedral	0	6	Octahedral	
Octahedral	1	5	Square Pyramidal	

Octahedral Parent Shape

Parent Shape	LP	BP	Molecular Shape	3D Structure
Octahedral	2	4	Square planar	
Octahedral	3	3	T-shape	
Octahedral	4	2	Linear	