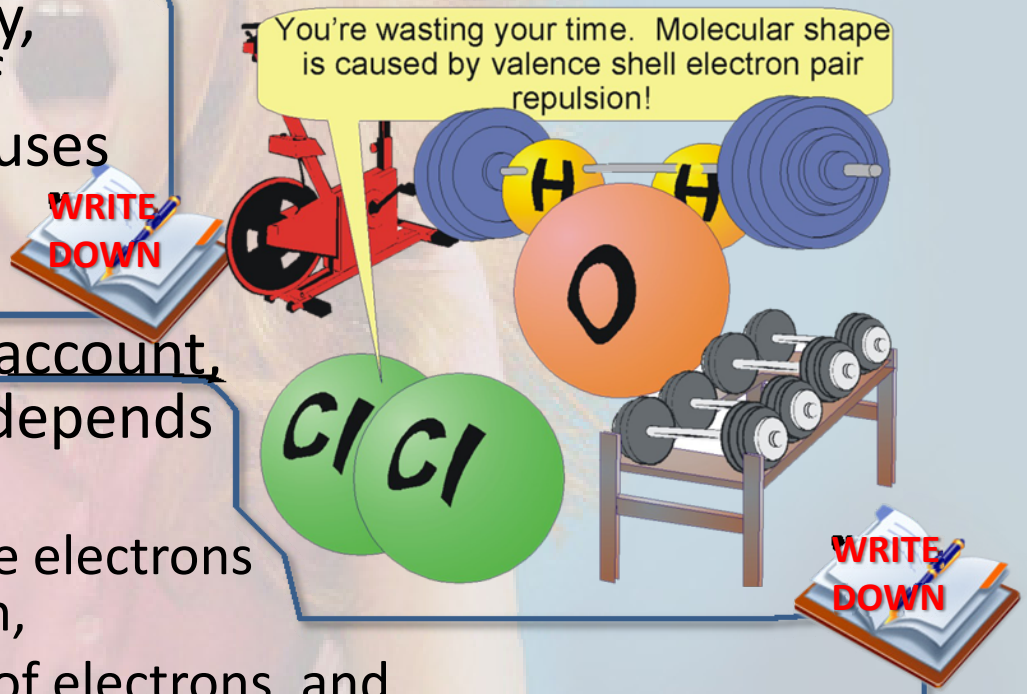
VSEPR

Valence Shell Electron Pair Repulsion

Predicting Molecular Shape

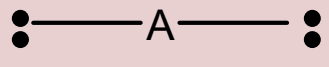
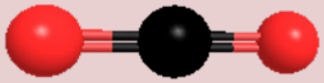
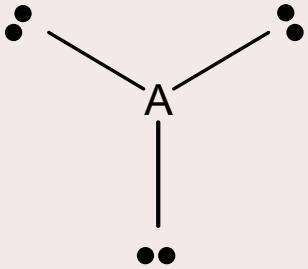
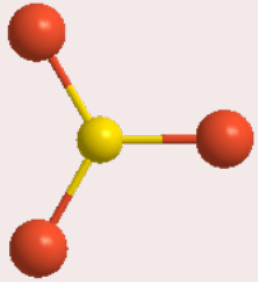
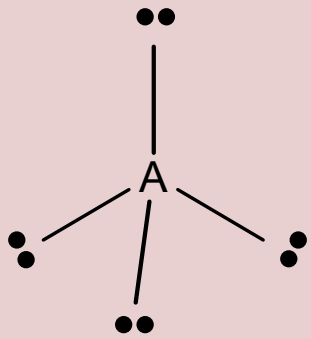
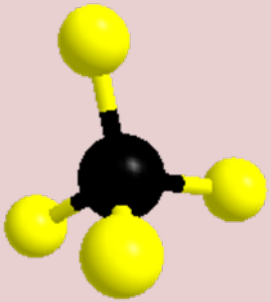
- One approach to predicting molecular shape is the valence shell electron pair repulsion model (VSEPR).
- According to VSEPR theory, repulsion between sets of valence shell electrons causes them to be as far apart as possible.
- Taking this repulsion into account, the shape of a molecule depends upon
  - how many pairs of valence electrons surround the central atom,
  - the number of lone pairs of electrons, and
  - the presence of multiple bonds (double bonds or tripe bonds).



VSEPR Rules

- Two pairs of valence electrons will be at 180˚ to each other producing a linear molecule
- Three pairs of valence electrons will be at 120˚ to each other in a single plane producing a trigonal planar molecule
- Four pairs will be at 109.5˚ to each other producing a tetrahedral molecule, a three sided pyramid with a triangular base.
  - The central atom is in the center of the pyramid
  - The attached atoms are at the four apices.
- Five pairs of valence electrons around the central atom produces a trigonal bipyramid, a molecule with a trigonal planar portion having bond angles of 120˚ and two bonding sites above and below the plane at 90˚ to it.
- Six pairs of valence electrons around the central atom produces an octahedral molecule with 90˚angles in all six directions.

VSEPR Rules Illustrated

Number of Electron Pairs	Shape	Arrangement of Electron Pairs		
2	Linear			
3	Trigonal planar			
4	Tetrahedral			

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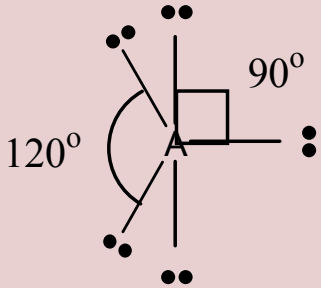
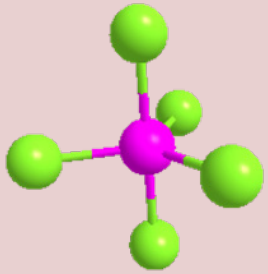
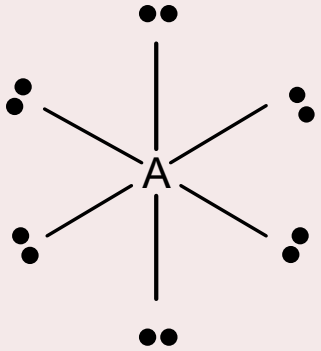
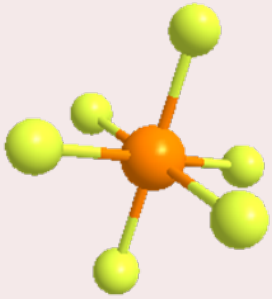
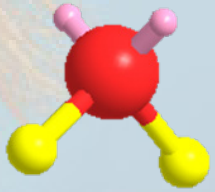
VSEPR Rules Illustrated (continued)

Number of Electron Pairs	Shape	Arrangement of Electron Pairs		
5	Trigonal bipyramidal			
6	Octahedral			

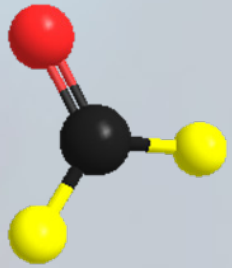
Other Considerations

- If the central atom and has a full octet of valence electrons, but some of them are lone pairs, the bond angle changes from the standard 109.5° tetrahedral angle.
  - Lone pairs of electrons increase the repulsion between electrons reducing the angle between bonded pairs.
  - The bond angle is smaller in water than in ammonia because it has two lone pairs of electrons instead of one.



= Lone Pair

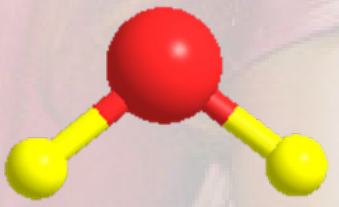
- Double and triple bonds are treated like single bonds.
  - As a result, CH_2O is trigonal planar



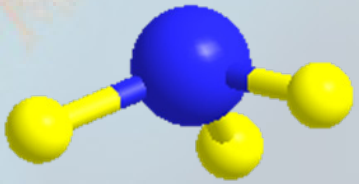
Tricky Tetrahedrons

- The electrons of water and ammonia are arranged around their central atoms at the four vertices of a tetrahedron, but the molecules are not tetrahedral.

- Only the actual atoms in the compound are part of the shape. The lone pairs are not.
- As a result:
  - Water is bent.
  - Ammonia is pyramidal



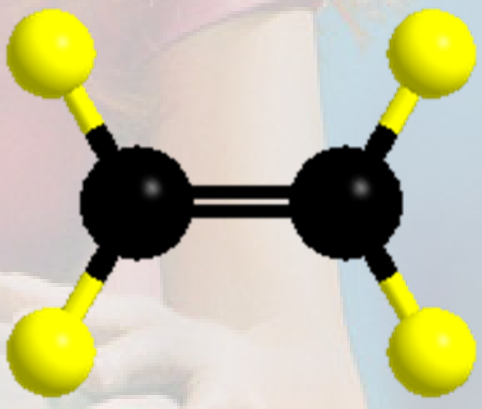
Water



Ammonia

Bigger Molecules

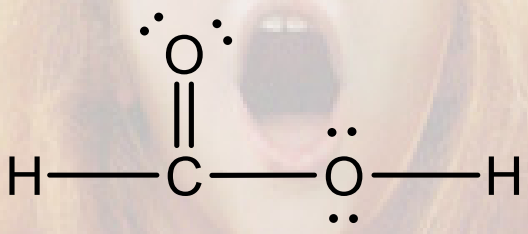
- For molecules in which there is no central atom, it is possible to predict the shape of sections of the molecule.
- In the molecule ethene (C_2H_4), for example, each of the carbons behaves like a central atom.
- The shape around each is trigonal planar.



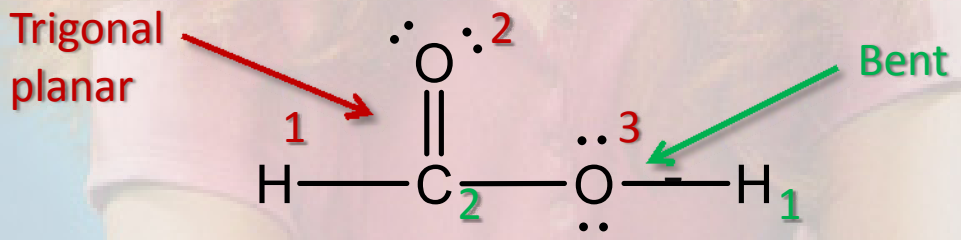
Sample Problem

What is the shape of CHOOH?

- **Step 1:** Draw the Lewis structure.



- **Step 2:** Count the number of electron pairs around the central atoms.



- Step 3: Identify the shapes around the central atoms.