

## Predicting Molecular Shapes

- the shape of a molecule is primarily determined by the behavior of valence electrons
- electron pairs want to be as far apart as possible (repulsive forces)

### VSEPR Theory

(Valence Shell Electron Pair Repulsion Theory)

- valence shell electron pairs want to stay as far apart as possible to minimize repulsive forces


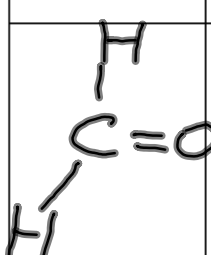
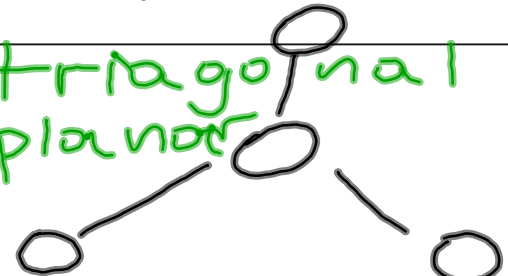
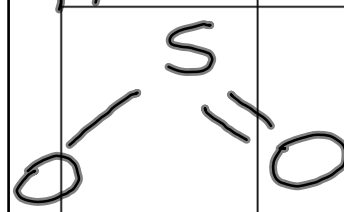
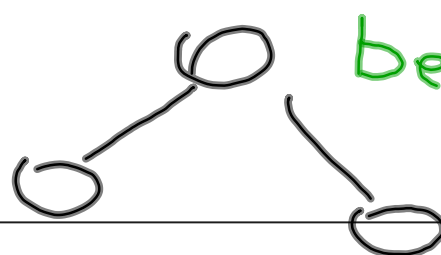
An electron pair is either:

- 1) a covalent bond
- 2) a lone pair

According to VSEPR theory:

- the shape of a molecule is determined by the number of covalent bonds and lone pairs around the central atom
- a double or triple bond counts as one electron pair around the central atom

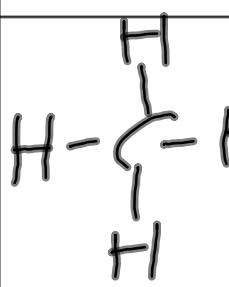
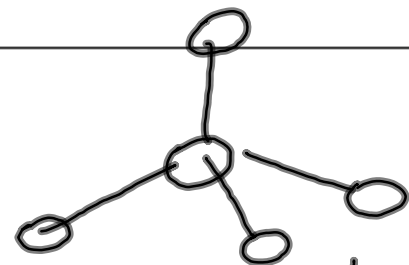
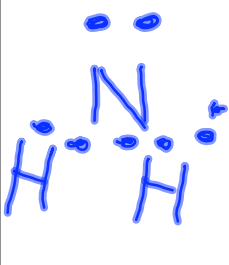

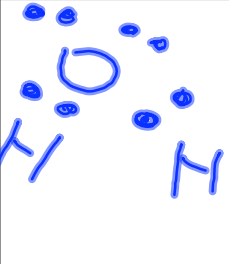
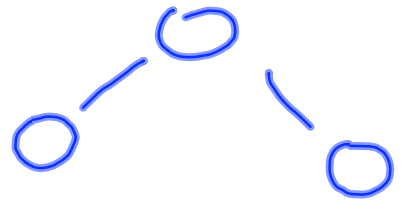
## Molecules With 4 Electron Pairs Around the Central Atom

Lewis Formula	# of Bonds	# of Lone Pairs	VSEPR Shape
$O=C=O$			 linear
			trigonal planar 
			bent 

AX<sub>2</sub>

Ex:

CO<sub>2</sub>AX<sub>3</sub>CH<sub>2</sub>OAX<sub>2</sub>SO<sub>2</sub>

Lewis Formula	# of Bonds	# of Lone Pairs	VSEPR Shape
	4	0	 tetrahedral $AX_4$ $CH_4$
	3	1	trigonal  pyramidal $EX_3$ $NH_3$
	2	2	 $H_2O$ Bent

## Chemistry 20 VSEPR Worksheet

1. According to VSEPR theory what determines the shape of a molecule?

e) HCl

f)  $\text{PO}_4^{3-}$ 

2. In order to make the rules of VSEPR work how must a multiple bond be treated?

g)  $\text{CO}_2$ 

h) HCN

3. What is the difference between a trigonal planar molecule and a trigonal pyramidal molecule?

4. Use Lewis Formulas and VSEPR theory to predict the shape of the following molecules:

i)  $\text{H}_2\text{CO}$ 

j) CO

a)  $\text{BeCl}_2$ b)  $\text{SiBr}_4$ k)  $\text{BrO}_3^-$ l)  $\text{C}_2\text{H}_6$ c)  $\text{PF}_3$ d)  $\text{BBR}_3$

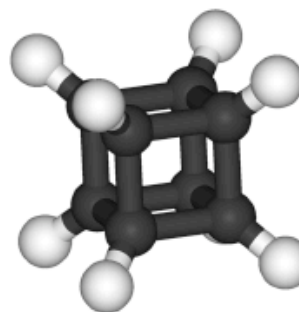
5. The predicted bond angle in a trigonal planar molecule is  $120^\circ$ . The observed bond angles in a molecule of  $\text{COCl}_2$  are  $124.5^\circ$  between the carbon chlorine and carbon oxygen bond and only  $111^\circ$  between the two carbon-chlorine bonds

a) Draw a structural formula for this molecule, including bond angles.

b) Provide a possible explanation for the deviation from predicted bond angles.

6. Cubane is a hydrocarbon with the formula  $\text{C}_8\text{H}_8$ , it has a cubic shape with a carbon atom at each corner of the cube. This molecule is very unstable, and some researchers have been seriously injured when crystals of the compound exploded while being scooped out of a bottle.

Cubane



a) According to VSEPR theory, what should be the shape around each carbon atom? Why?

b) If we assume an ideal cubic shape in cubane, what are the actual bond angles around each carbon?

c) Explain how your answers to a) and b) suggest why this molecule is so unstable.