## CHM151LL: VSEPR and Molecular Geometry Tables

VALENCE-SHELL ELECTRON-PAIR REPULSION (VSEPR) MODEL
Lewis structures show the two-dimensional distribution of atoms and electrons. The molecular geometry, or three-dimensional shape of a molecule or polyatomic ion, can be determined using valence-shell electron-pair repulsion (abbreviated VSEPR and pronounced "VES-per") theory, in which the basic principle is valence electrons around a central atom stay as far apart as possible to minimize the repulsions.

For diatomic molecules (i.e., those made up of two atoms), the shape has to be linear. For molecules with three of more atoms, the shape depends on the number and type of electrons (bonding versus nonbonding) around the central atom. Since electrons are negatively charged and repel one another, electrons on the central atom of a molecule always maximize their distance from one another. These repulsions give rise to the five basic molecular geometries (or shapes) for molecules in which the central atom has no lone pairs. These shapes are described below.

## Basic Molecular Geometries (or Shapes) where the Central Atom has No Lone Pairs

Consider a molecule composed of only two types of atoms, A and B:

## $A=$ central atom $\quad B=o u t e r$ atoms

For three or more atoms in a molecule, general formula: $\mathbf{A B}_{\#}$ (where \#=2-6)

## $\mathrm{AB}_{2}$ : linear

- the two outer atoms are $\mathbf{1 8 0}^{\circ}$ from each other


## $\mathrm{AB}_{3}$ : trigonal planar

- three outer atoms at the corners of an equilateral triangle
- each outer atom is $\mathbf{1 2 0}^{\circ}$ from the other two outer atoms
$\mathbf{A B}_{4}$ : tetrahedral (tetra $=$ four) since four-sided, or four faces
- maximum distance between electrons requires 3D structure with
$109.5^{\circ}$ between each outer atom
- each outer atom is $109.5^{\circ}$ from the other outer atoms
$\mathrm{AB}_{5}$ : trigonal bipyramidal
- trigonal = three outer atoms form planar triangle around central atom
- bipyramidal = two outer atom directly above and below central atom, connecting outer atom forms two 3-sided pyramids
- equatorial positions: corners of planar triangle
- 3 of outer atoms are at equatorial positions, $\mathbf{1 2 0}^{\circ}$ from each other
- axial positions: above and below central atom
-2 atoms are at axial positions, $9 \mathbf{0}^{\circ}$ from equatorial atoms
AB $_{6}$ : octahedral (octa=eight) connecting the B atoms $\rightarrow$ eight faces
- all outer atoms are $90^{\circ}$ away from each other
- the terms "axial" and "equatorial" do not apply because all six positions are identical since the molecule is completely symmetrical


Molecular Geometries (or Shapes) where the Central Atom Does Have Lone Pairs
Predicting the shape of molecules where the central atom has lone pairs is somewhat more difficult. Even though the lone pairs cannot be seen, they are still electrons which repel the bonding pairs of electrons. In fact, they are actually more repulsive than bonding pairs, so they compress the bond angles in the molecules where they are present. For molecules where the central atom has lone pairs, we can write a general formula that also includes the lone pairs represented by the letter E, as shown below.
$A=$ central atom $\quad B=o u t e r$ atoms $\quad E=l o n e$ pairs on the central atom
The various molecular geometries for these types of molecules are shown in tables and described on the following pages:

## Molecular Geometries Where Central Atom Has Lone Pairs (Continued)

| Original Shape without Lone Pairs | \# of Outer Atoms | \# of Lone Pairs | General <br> Formula | Molecular Geometry | Name |
| :---: | :---: | :---: | :---: | :---: | :---: |
| trigonal planar ( $\mathrm{AB}_{3}$ ) | 2 | 1 | $\mathrm{AB}_{2} \mathrm{E}$ |  | bent or angular |
|  | 3 | $1$ <br> 2 | $\mathrm{AB}_{3} \mathrm{E}$ <br> $\mathrm{AB}_{2} \mathrm{E}_{2}$ |  | trigonal pyramidal <br> bent or angular |

Molecular Geometry from Trigonal Planar
$\mathrm{AB}_{2} \mathrm{E}$ : bent

- start with $\mathrm{AB}_{3}$ molecule (trigonal planar) and replace a $B$ atom w/ lone pair
- lone pair electrons push bonding electrons away
$\rightarrow$ bond angles are now less than $\mathbf{1 2 0}{ }^{\circ}$


## Molecular Geometries from Tetrahedral

$\mathbf{A B}_{3} \mathrm{E}$ : trigonal pyramidal (central atom +3 outer atoms make a pyramid)

- start with $\mathrm{AB}_{4}$ molecule (tetrahedral) and replace a $\mathbf{B}$ atom w/ lone pair
- lone pair electrons push bonding electrons away $\rightarrow$ bond angles are now less than $109 . \mathbf{5}^{\circ}$


## $\mathrm{AB}_{2} \mathrm{E}_{2}$ : bent

- start with $\mathrm{AB}_{4}$ molecule (tetrahedral) and replace $2 \mathbf{B}$ atoms with 2 lone pairs
- lone pair electrons repel each other and the bonding electrons $\rightarrow$ bond angles are now less than $109 . \mathbf{5}^{\circ}$


## Molecular Geometries from Trigonal Bipyramidal

## $\mathrm{AB}_{4} \mathrm{E}$ : seesaw

- start with $A B_{5}$ molecule and replace one $B$ atom with one lone pair
- a B atom can be taken from an axial or an equatorial position - from axial: lone pair is $90^{\circ}$ from three equatorial $B$ atoms and
- from equatorial: lone pair is $90^{\circ}$ from two Axial and $120^{\circ}$ from two other equatorial B atoms
- taking a B atom from equatorial position maximizes space between lone pair and $B$ atoms
- lone pair electrons push bonding electrons away
$\rightarrow$ bond angles are now less than $\mathbf{9 0}^{\circ}$ and less than $\mathbf{1 2 0}{ }^{\circ}$


## $\mathrm{AB}_{3} \mathrm{E}_{2}$ : T-shaped

- start with $\mathrm{AB}_{5}$ molecule and replace two B atoms with two lone pairs
- both B atoms taken from equatorial positions to maximize distance between the lone pairs
- lone pair electrons repel each other and the bonding electrons $\rightarrow$ bond angles for remaining atoms are now less than $\mathbf{9 0}^{\circ}$


## $\mathrm{AB}_{2} \mathrm{E}_{3}$ : linear

- start with $A B_{5}$ molecule and replace three $B$ atoms with three lone pairs
- taking three $B$ atoms from equatorial positions maximizes space between the $\backslash$ lone pairs, keeping them $120^{\circ}$ from one another
- lone pair electrons repel each other and the bonding electrons, but since the bonding electrons are balanced on either side of the 3 lone pairs $\rightarrow$ bond angle is exactly $180^{\circ}$


## Molecular Geometries Where Central Atom Has Lone Pairs (Continued)

| Original Shape without Lone Pairs | \# of Outer Atoms | $\begin{gathered} \text { \# of Lone } \\ \text { Pairs } \end{gathered}$ | General Formula | Molecular Geometry | Name |
| :---: | :---: | :---: | :---: | :---: | :---: |
| trigonal bipyramidal $\left(\mathrm{AB}_{5}\right)$ | 4 | 1 | $\mathrm{AB}_{4} \mathrm{E}$ |  | See-saw |
|  | 3 | 2 | $\mathrm{AB}_{3} \mathrm{E}_{2}$ |  | T-shaped |
|  | 2 | 3 | $\mathrm{AB}_{2} \mathrm{E}_{3}$ |  | linear |

Molecular Geometries from Octahedral
$\mathbf{A B}_{5} \mathbf{E}$ : square pyramidal (central atom +5 B atoms make 4-faced pyramid)

- start with $\mathrm{AB}_{6}$ (octahedral) and replace one $B$ atom with one lone pair
- all six outer positions are identical, so any outer atom can be removed
$\rightarrow$ square pyramidal shape
- lone pair electrons push bonding electrons away
$\rightarrow$ bond angles are now less than $\mathbf{9 0}^{\circ}$
$\mathbf{A B}_{4} \mathbf{E}_{2}$ : square planar (central atom +4 B atoms form square all in 1 plane)
- start with $\mathrm{AB}_{6}$ (octahedral) and replace 2 B atoms with 2 lone pairs
- remove first B atom then remove the second B atom $180^{\circ}$ away from the first to maximize the distance between the lone pairs
$\rightarrow$ square planar shape
- bond angles are now exactly $\mathbf{9 0}^{\circ}$ since lone pairs balance each other

Molecular Geometries Where Central Atom Has Lone Pairs (Continued)

| Original Shape without Lone Pairs | \# of <br> Outer <br> Atoms | \# of <br> Lone <br> Pairs | General <br> Formula | Molecular Geometry | Name |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | 5 | 1 | $\mathrm{AB}_{5} \mathrm{E}$ |  | square pyramidal |
|  | 4 | 2 | $\mathrm{AB}_{4} \mathrm{E}_{2}$ |  | square <br> planar |

