CHM151LL: VSEPR and Molecular Geometry Tables

VALENCE-SHELL ELECTRON-PAIR REPULSION (VSEPR) MODEL 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 B=outer atoms
For th	ree or more atoms in a molecule, general formula: $AB_{\#}$ (where $\#=2-6$)
AB ₂ :	linearthe two outer atoms are 180° from each other
AB ₃ :	 trigonal planar three outer atoms at the corners of an equilateral triangle each outer atom is 120° from the other two outer atoms
AB ₄ :	 tetrahedral (<i>tetra</i> = four) since four-sided, or four faces maximum distance between electrons requires 3D structure with 109.5° between each outer atom each outer atom is 109.5° from the other outer atoms
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, 120° from each other
	 axial positions: above and below central atom 2 atoms are at axial positions, 90° from equatorial atoms
AB ₆ :	octahedral (<i>octa</i> =eight) connecting the B atoms \rightarrow eight faces

- all outer atoms are 90° away from each other
 - the terms "axial" and "equatorial" do not apply because all six positions are identical since the molecule is completely symmetrical

# of Outer Atoms	General Formula	Molecular Geometry and Bond Angles	Name
2	AB ₂		linear
3	AB ₃		trigonal planar
4	AB ₄	109.5°	tetrahedral
5	AB ₅	90° 90° 120°	trigonal bipyramidal
6	AB ₆	90°	octahedral

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 B=outer atoms E=lone 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 Formula	Molecular Geometry	Name
trigonal planar (AB ₃)	2	1	AB ₂ E	<120°	bent or angular
tetrahedral (AB ₄) 109.5°	3	1	AB3E	<109.5°	trigonal pyramidal
	2	2	AB_2E_2	<109.5°	bent or angular

Molecular Geometry from Trigonal Planar

AB₂E: bent

- start with AB₃ 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 120°

Molecular Geometries from Tetrahedral

AB₃E: trigonal pyramidal (central atom + 3 outer atoms make a pyramid)

- start with AB_4 molecule (tetrahedral) and replace a B atom w/ lone pair
- lone pair electrons push bonding electrons away
 - \rightarrow bond angles are now less than 109.5°

AB₂E₂: bent

- start with AB₄ molecule (tetrahedral) and replace **2 B atoms** with **2 lone pairs**
- lone pair electrons repel each other and the bonding electrons
 - \rightarrow bond angles are now less than 109.5°

Molecular Geometries from Trigonal Bipyramidal

AB₄E: seesaw

- start with AB₅ 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° from three equatorial B atoms and
 - from equatorial: lone pair is 90° from two Axial and 120° 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 90° and less than 120°

AB₃E₂: T-shaped

- start with 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 90°

AB₂E₃: linear

- start with AB₅ molecule and replace three B atoms with three lone pairs
- taking three B atoms from equatorial positions maximizes space between the $\$ lone pairs, keeping them 120° 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**°

Original Shape without Lone Pairs	# of Outer Atoms	# of Lone Pairs	General Formula	Molecular Geometry	Name
trigonal bipyramidal	4	1	AB₄E	<90°	See-saw
(AB ₅) 90° 120°	3	2	AB ₃ E ₂	<90°	T-shaped
	2	3	AB ₂ E ₃		linear

Molecular Geometries Where Central Atom Has Lone Pairs (Continued)

Molecular Geometries from Octahedral

AB₅E: square pyramidal (central atom + 5 B atoms make 4-faced pyramid)

- $-\,$ start with 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
 → square pyramidal shape
- lone pair electrons push bonding electrons away
 - \rightarrow bond angles are now less than 90°

AB₄E₂: square planar (central atom + 4 B atoms form square all in 1 plane) start with AB (satchedrel) and we have 2B stores with 2 large pairs

- start with AB_6 (octahedral) and replace **2 B atoms** with **2 lone pairs**
- remove first B atom then remove the second B atom 180° away from the first to maximize the distance between the lone pairs
 - \rightarrow square planar shape
- bond angles are now exactly 90° since lone pairs balance each other

Original Shape without Lone Pairs	# of Outer Atoms	# of Lone Pairs	General Formula	Molecular Geometry	Name
octahedral (AB ₆)	5	1	AB5E	90°	square pyramidal
	4	2	AB ₄ E ₂	9000000	square planar

Molecular Geometries Where Central Atom Has Lone Pairs (Continued)