

## I. Chapter 9 Molecular Geometry and Bonding Theories

- The shape and size of molecules is sometimes referred to as *molecular architecture*-defined by the angles and distances between the nuclei of the component atoms.
- Properties of a substances are largely determined by shape, size, and strength of bonds and polarity of bonds.
- Shape of a molecule is governed by the kinds of bonds that exist between the atoms making up a molecule.


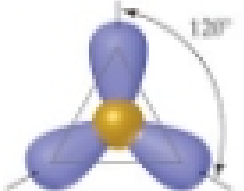
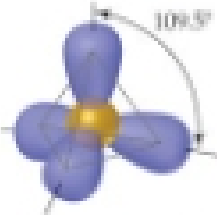
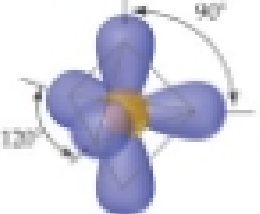
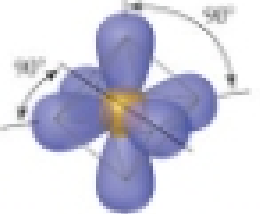
### A. 9.1 Molecular Shapes

- Lewis structures do not indicate shape of molecules; they show the number and type of bonds.
- A *tetrahedron* is a geometric object with four corners and four faces, each an equilateral triangle.
- The shape of a molecule is determined by its **bond angles**, the angles made by the lines joining the nuclei of the atoms in a molecule.
- Bond angles and bond length together define the shape and size of the molecule.
- Molecular shapes with molecules or ions that have a single central atom bonded to two or more atoms of the same element have the general formula  $AB_n$  in which the central atom A is bonded to n B atoms.
- The number of shapes possible for  $AB_n$  molecules depends on the value n.
- A  $AB_2$  must either be linear (bond angle =  $180^\circ$ ) or bent (bond angle  $\neq 180^\circ$ ).
- For  $AB_3$  molecules, the two most common shapes place the B atom at the corners of an equilateral triangle.
- For  $AB_3$  molecules, if the A atom lies in the same plane as the B atoms, the shape is *trigonal planer*.
- For  $AB_3$  molecules, if the A atom lies above the plane of the B atoms, the shape is *trigonal pyramidal* (a pyramid with an equilateral triangle as its base).
- Some  $AB_3$  molecules are *T-shaped*; a relatively unusual shape where all the atoms lie in one plane, but the angles between them vary.
- The *trigonal bipyramidal* can be thought of as two face-to-face *trigonal pyramids*; the *octahedron* is like to face-to-face *square pyramids*.
- When A is a representative element (one from the s block or p block of the periodic table), we can predict the shapes by using **the valence-shell electron-pair repulsion (VSEPR) model**.

### B. 9.2 The VSEPR Model

- A **bonding pair** of electrons defines a region in which electrons are most likely to be found.
- This region of space where electrons are most likely to be found is referred to as an **electron domain**.
- A **nonbonding pair** (or **lone pair**) of electrons defines an electron domain that is located principally on one atom.
- Each multiple bond in a molecule constitutes a single domain.









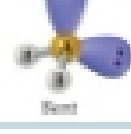
TABLE 9.1 Electron-Domain Geometries as a Function of the Number of Electron Domains

Number of Electron Domains	Arrangement of Electron Domains	Electron-Domain Geometry	Predicted Bond Angles
2		Linear	180°
3		Trigonal planar	120°
4		Tetrahedral	109.5°
5		Trigonal bipyramidal	120° 90°
6		Octahedral	90°

- In general, each nonbonding pair, single bond, or multiple bond produces a single electron domain around the central atom in a molecule.
- The best arrangement of a given number of electron domains is the one that minimizes the repulsions among them.

- The shapes of different  $AB_n$  molecules or ions depend on the number of electron domains surrounding the central atom.
- The arrangement of electron domains about the central atom of an  $AB_n$  molecule or ion is called its **electron-domain geometry**.
- The **molecular geometry** is the arrangement of *only the atoms* in a molecule or ion- any nonbonding pairs in the molecule are *not* part of the description of the molecular geometry.
- When all the electron domains in a molecule arise from bonds, the molecular geometry is identical to the electron domain geometry.
- When one or more domains involve nonbonding pairs of electrons, we must remember to ignore those domains when talking about molecular shape.
- The generalized steps for using the VSEPR model to predict shapes of molecules or ions:
  1. Draw the *Lewis structure* of the molecule or ion and count the number of electron domains around the central atom.
  2. Determine the *electron-domain geometry* by arranging the electron domains about the central atom so that the repulsions among them are minimized.
  3. Use the arrangements of the bonded atoms to determine the *molecular geometry*.

TABLE 9.2 Electron Domain Geometries and Molecular Shapes for Molecules with Two, Three, and Four Electron Domains Around the Central Atom

Number of Electron Domains	Electron-Domain Geometry	Bonding Domains	Nonbonding Domains	Molecular Geometry	Example
2		2	0		$CO_2$
3		3	0		$BF_3$
		2	1		$SO_2$
4		4	0		$CH_4$
		3	1		$NH_3$
		2	2		$H_2O$

## 1. Effect of Nonbonding Electrons and Multiple Bonds on Bond Angles

- Bond angle decreases as the number of nonbonding electron pairs increases.
- A bonding pair of electrons is attracted by both nuclei of the bonded atoms, but a nonbonding pair is attracted primarily by only one nucleus.
- Because a nonbonding pair experiences less nuclear attraction, its electron domain is spread out more in space than is the electron domain for a bonding pair.
- *Electron domains for nonbonding electron pairs exert greater repulsive forces on adjacent electron domains and tend to compress bond angles.*
- Because multiple bonds contain higher

electronic-charge density than single bonds, multiple bonds also represent enlarged electron domains.

- In general, *electron domains for multiple bonds exert a greater repulsive force on adjacent electron domains than do electron domains for single bonds.*

## 2. Molecules with Expanded Valence Shells

- Atoms from period three may be surrounded by more than four electron pairs.