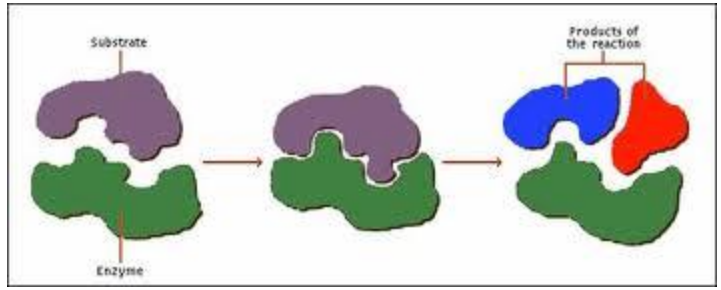
Three Dimensional Structure

Chapter 4.2

Molecular Geometry

- The Lewis Structure provided some insight into molecular structure in terms of **bonding**, but what about **geometry**?
- Knowing the **three-dimensional** structure of a molecule helps us to make predictions about its properties



The VSEPR Theory

- **Valence Shell Electron Pair Repulsion (VSEPR)** Theory is a method used to determine the geometry of a molecule:
  - Atoms can have two types of electron pairs **bonding pairs** and **lone pairs**
  - Electrons are all **negatively** charged and thus **repel** each other
  - Electrons position themselves as **far apart** as possible in a molecule to minimize the repulsive forces between them

Let’s Give it a Try!

- Draw the Lewis structure and determine the shape of:

a) BeF_2

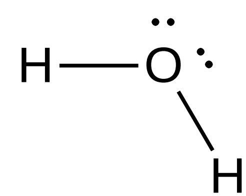
b) BF_3

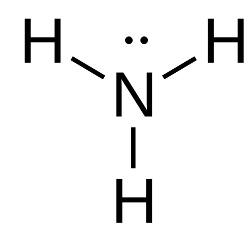
c) CF_4

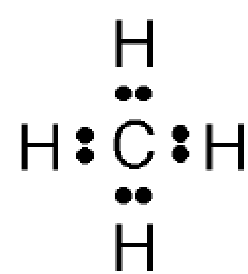
AXE Notation

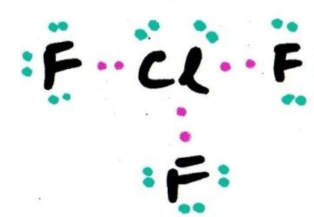
- One method of helping to understand molecular shapes is the AX_yE_z notation:
  - **A** denotes the central atom of the molecule
  - **X_y** shows how many terminal atoms are around the central atom
  - **E_z** shows how many lone pairs of electrons are around the central atom

Examples:



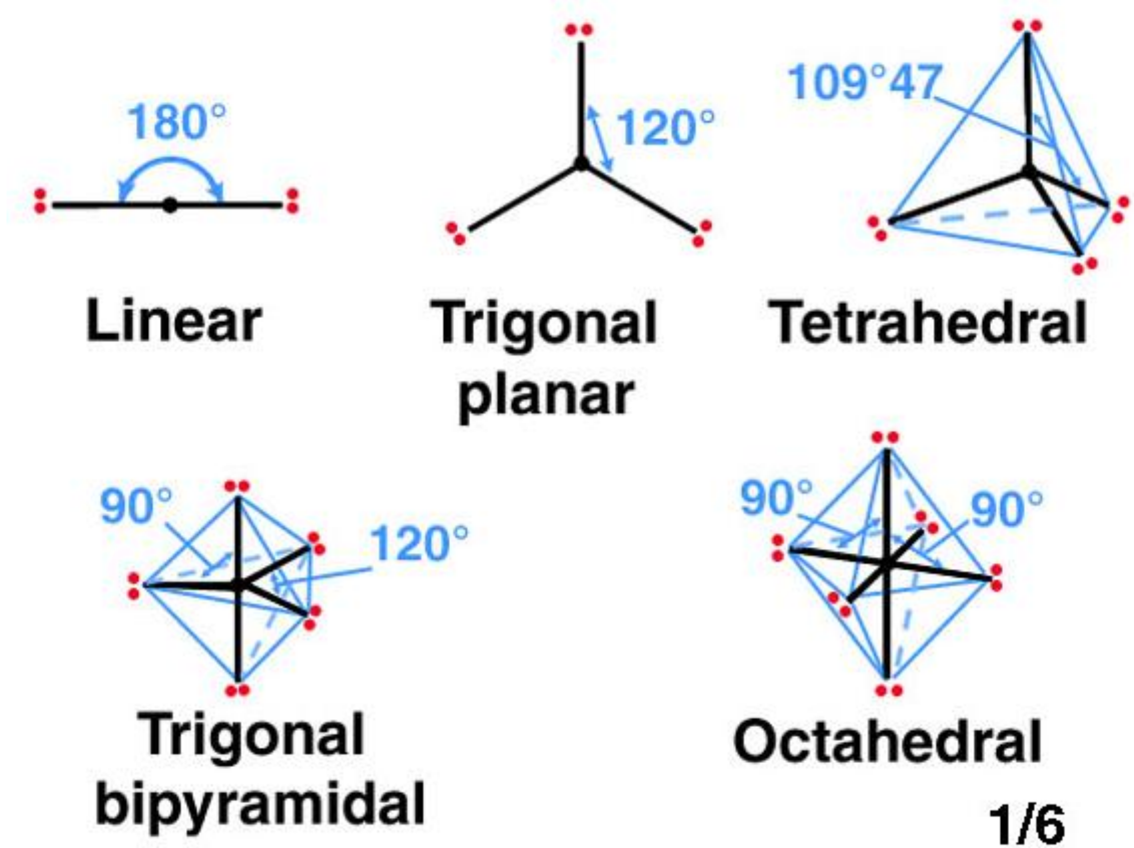




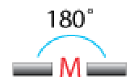
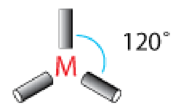
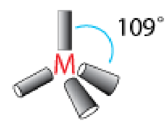
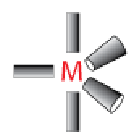
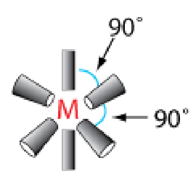


Main Shapes

All of these shapes are **symmetrical**

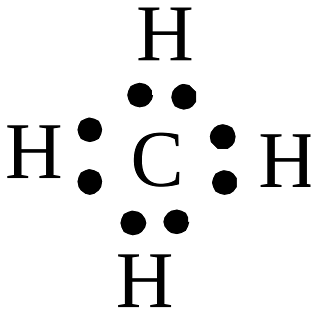


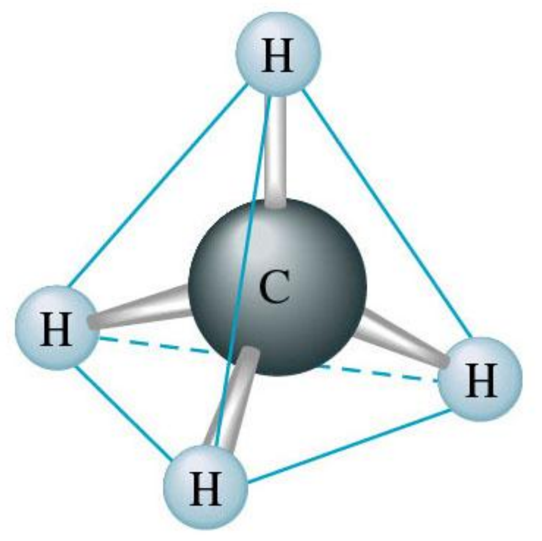
Main Shapes

# electron domains (bonding or non-bonding electron regions)	Structure	Name
2		linear
3		Trigonal Planar
4		Tetrahedral
5		Trigonal Bipyramidal
6		Octahedral

Variations on the Main Shapes

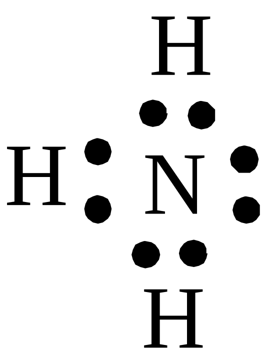
- Recall:
- Methane (CH_4) has 4 bonding pairs of electrons and a tetrahedral structure

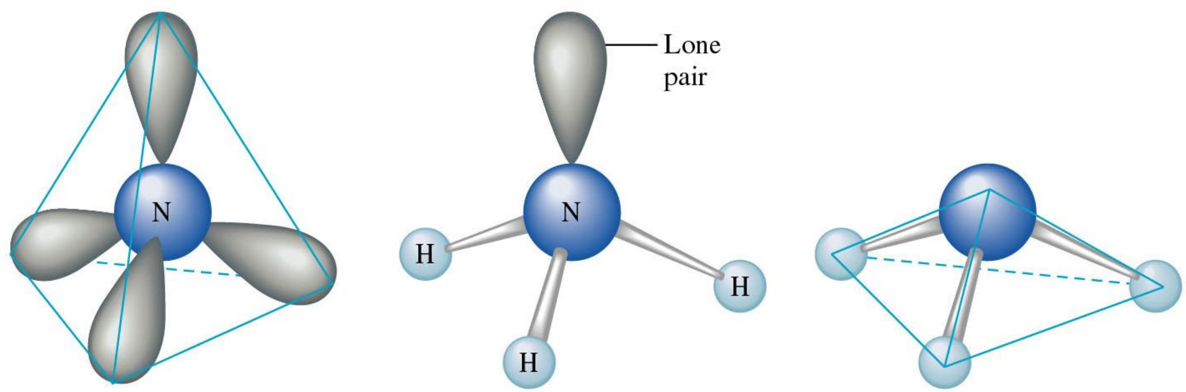




Variations on the Main Shapes

- **Ammonia (NH_3)** is similar to methane in the sense that it is surrounded by *four electron pairs*
- Unlike methane, *one* of ammonia's electron pairs is a *lone pair*
- This affects the overall VSEPR shape of the ammonia molecule

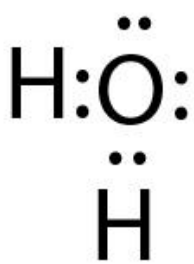


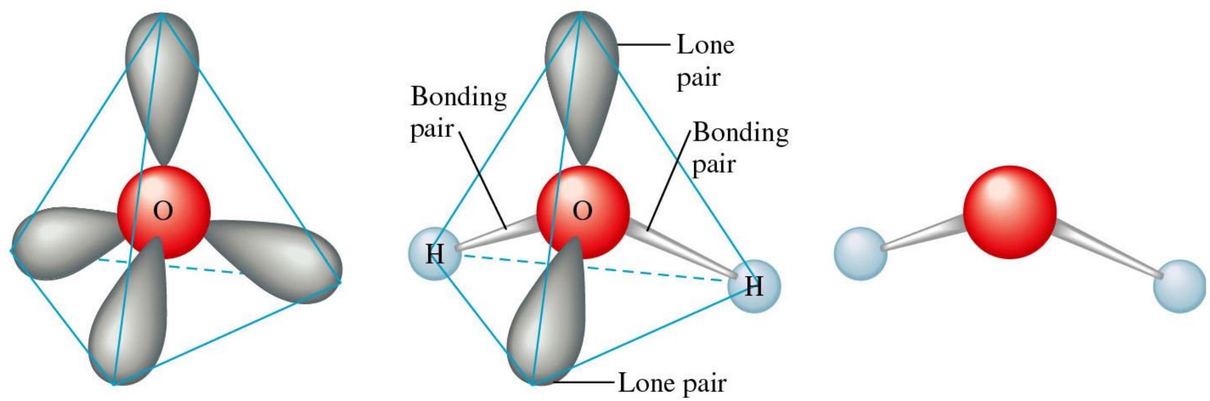


(a) (b) (c)

Variations on the Main Shapes

- **Water (H_2O)** is also similar to methane in the sense that it is surrounded by *four electron pairs*
- Unlike methane, *two* of water's electron pairs are *lone pairs*
- This affects the overall VSEPR shape of the water molecule

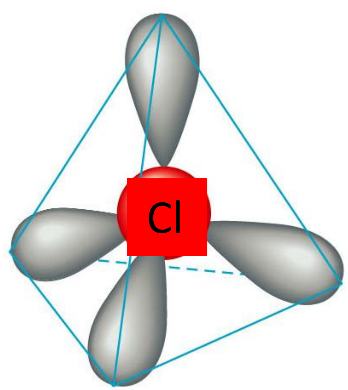




(a) (b) (c)

Variations on the Main Shapes

- We could take this one step further and consider the structure of hydrochloric acid
- **HCl** is also similar to methane in the sense that it is surrounded by *four electron pairs*
- Unlike methane, *three* of hydrochloric acid's electron pairs are *lone pairs*
- This affects the overall VSEPR shape of the water molecule

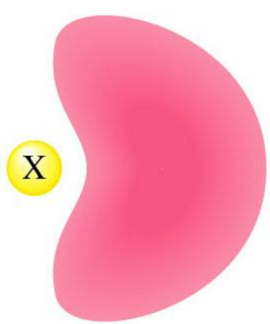


Variations on the Main Shapes

- The angle of the main shape may vary due to the size differences between bonding pair and lone pair electron densities

(a)

BONDING PAIR

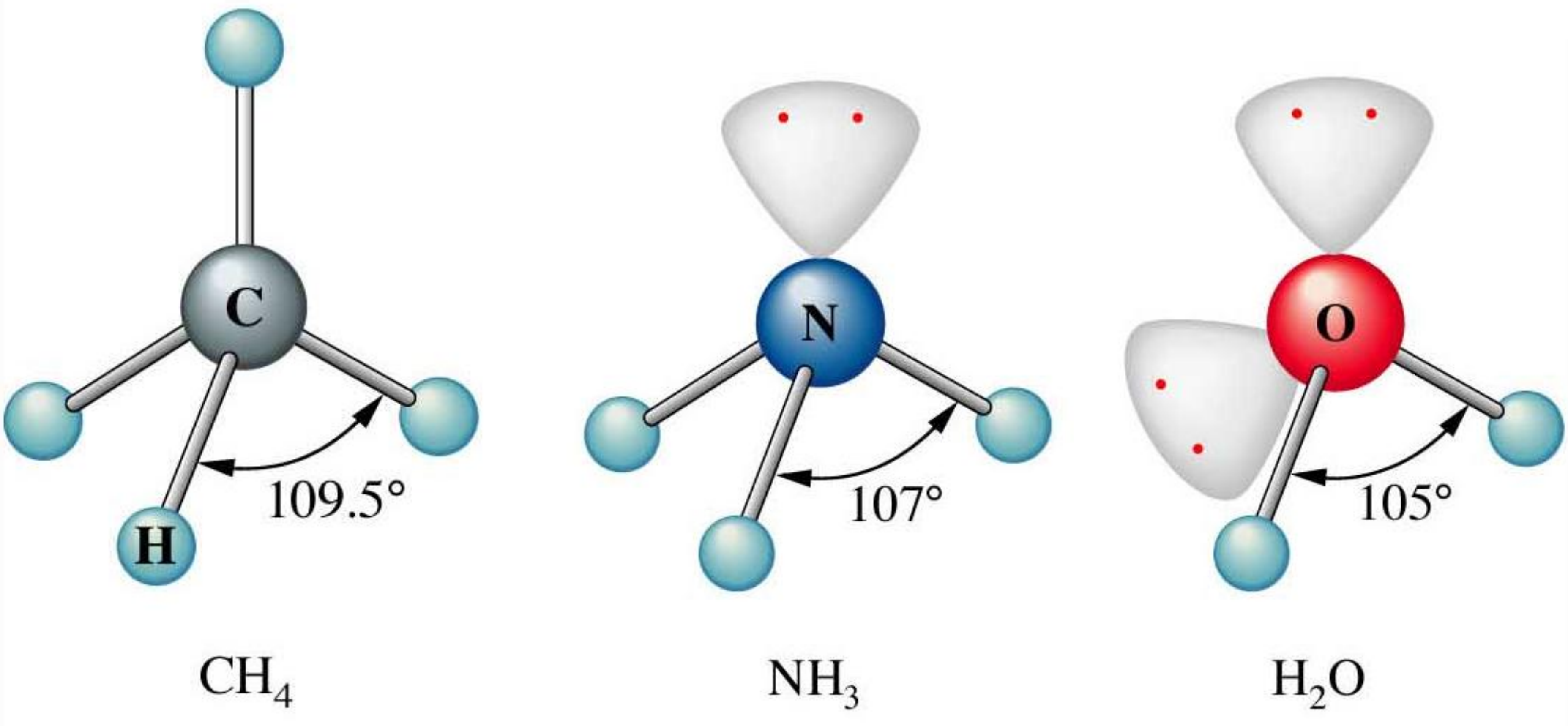


(b)

LONE PAIR

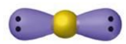
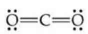
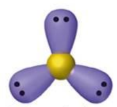
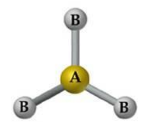
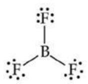
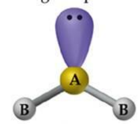
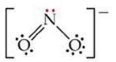
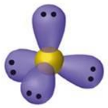
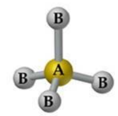
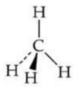
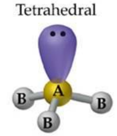
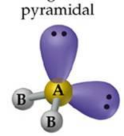
Variations on the Main Shapes

- The angle of the main shape may vary due to the size differences between bonding pair and lone pair electron densities
- Compare methane, ammonia, and water:



Variations on the Main Shapes

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	 Linear	2	0	 Linear	
3	 Trigonal planar	3	0	 Trigonal planar	
		2	1	 Bent	
4	 Tetrahedral	4	0	 Tetrahedral	
		3	1	 Trigonal pyramidal	
		2	2	 Bent	

Steps for Applying the VSEPR Theory:

1. Draw the correct Lewis Structure
2. Count the electron pairs surrounding the central atom (including both bonding pairs and lone pairs), and arrange them in a way that minimizes electron-pair repulsion (as far apart as possible in three dimensional space)
3. Place the atoms bonded to the central atom at the ends of their bonded electron pairs
4. Determine the name of the structure from the positions of the atoms and lone pairs of electrons

Practice

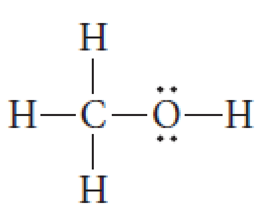
- Predict the VSEPR shape of BrF_5

More Than One Central Atom

- If the molecule has more than one central atom:

1. Predict the arrangement of electrons around each central atom individually
2. Combine these arrangements to predict the overall structure

Example: predict the structure of methanol (CH_3OH):



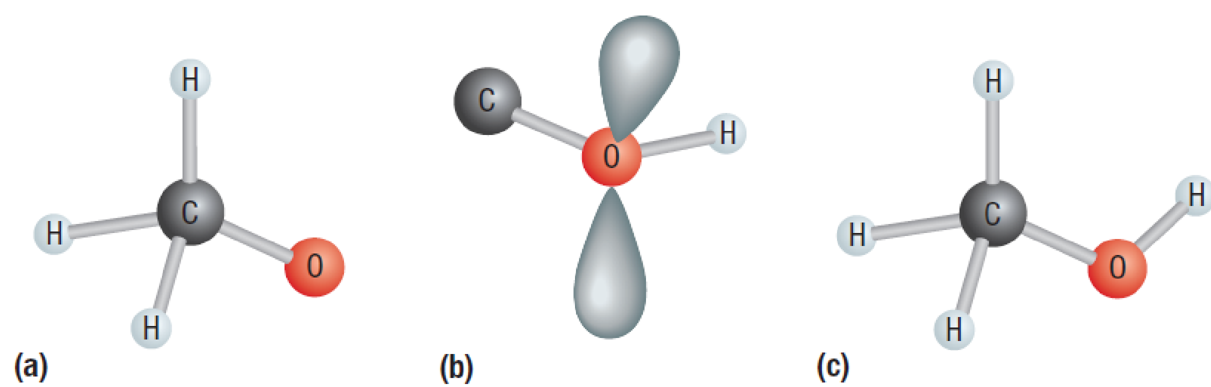
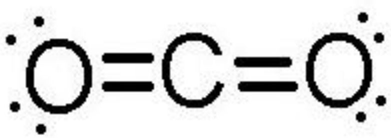
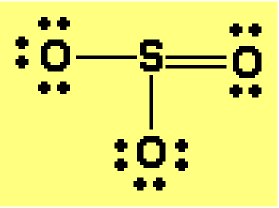


Figure 5 (a) The arrangement of atoms around the carbon atom is tetrahedral. (b) The arrangement of atoms and lone electron pairs around the oxygen atom is bent. (c) The three-dimensional structure of methanol.

Multiple Bonds

- If the molecule has double or triple bonds count them all together





Practice

- Use VSEPR theory to predict the shape of propene

VSEPR Theory Limitations

- VSEPR theory correctly predicts the structures of many molecules
- There are a few exceptions

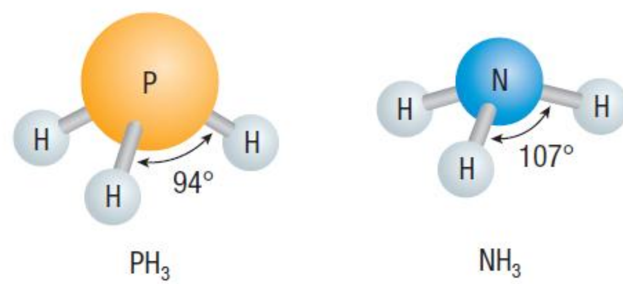


Figure 6 Even though phosphine has the same three-dimensional structure as ammonia, the angles between bonding atoms in the molecules are different: 94° in phosphine and 107° in ammonia.

HOMEWORK

Required Reading:

p. 206-216

(remember to supplement your notes!)

Questions:

p. 212 #1-2

p. 215 #1-2

p. 216 #1-10