Molecules Module – Lecture 3:
VSEPR Theory and The Shapes of Molecules

Learning Objective	Openstax 2e Chapter
VSEPR Theory	**7.6**

Suggested Practice Problems

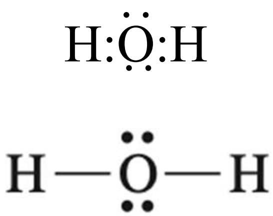
Chapter 7 Exercises – Questions: 85, 91, 93, 95, 105, 109

Answers can be found in the Chapter 7 Answer Key

Shapes of Molecules

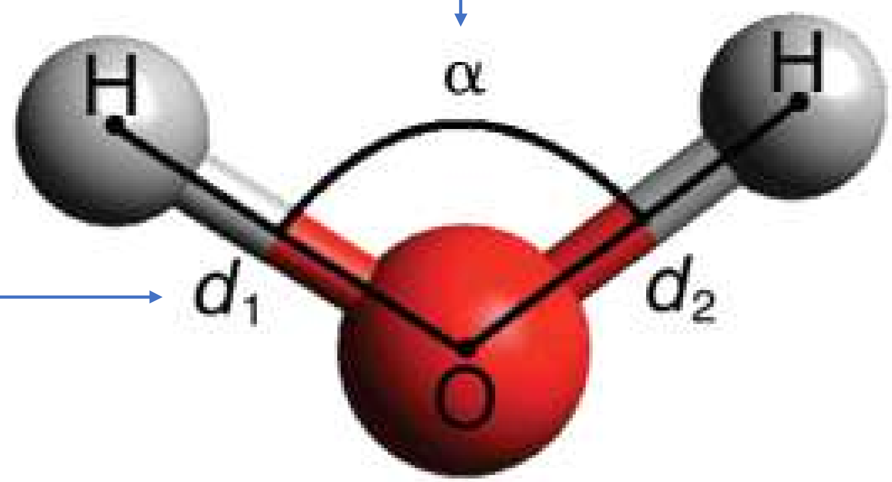
The geometric figure obtained when joining the nuclei of bonded atoms by straight lines.

Water, H_2O



Bond angle
angle between adjacent bonds

Bond length
distance between directly bonded nuclei



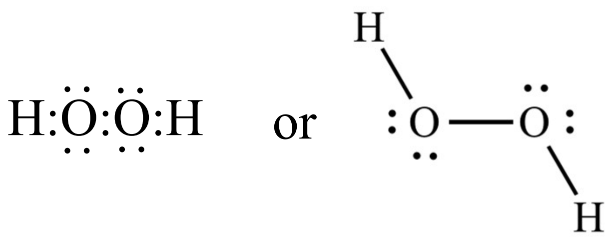
$\alpha = 104.45°$
$d_1 = d_2 = 95.8$ pm

Figure1: Geometrical shape water

Shapes of Molecules

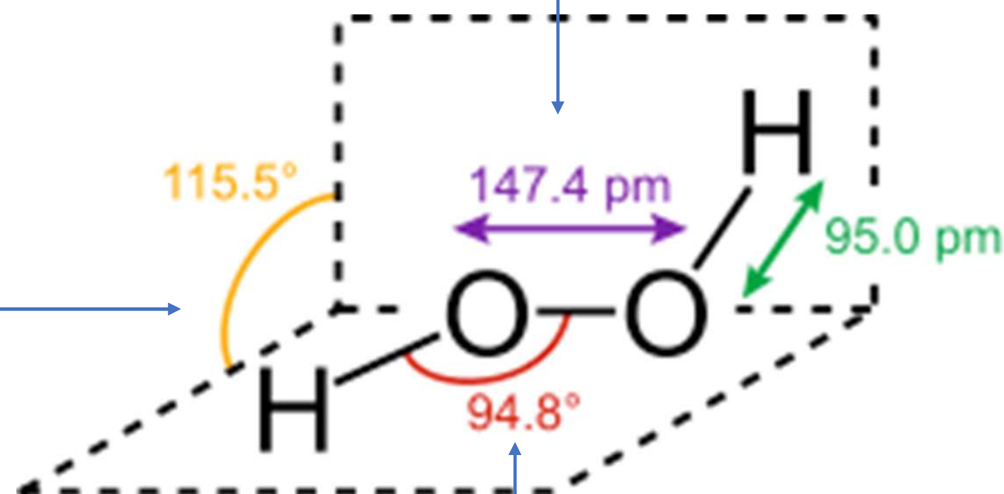
The geometric figure obtained when joining the nuclei of bonded atoms by straight lines.

Hydrogen peroxide, H_2O_2



Bond length
distance between directly bonded nuclei

Torsional angle (dihedral angle)
angle between two bond vectors



Bond angle
angle between adjacent bonds

Valence-Shell Electron Pair Repulsion (VSEPR) Theory

Electron pairs repel each other, whether they are in chemical bonds (bond pairs) or unshared (lone pairs). Electron pairs assume orientations about an atom to minimize repulsions.

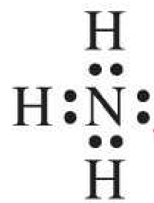
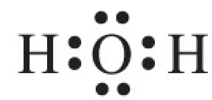
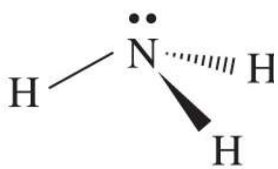
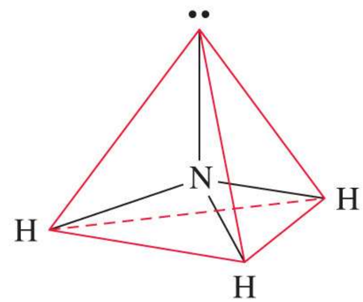
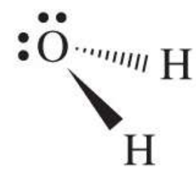
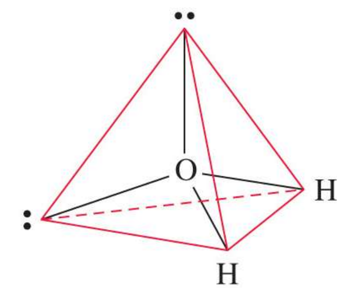
Repulsion Trend:

lone pair – lone pair > lone pair – bond pair > bond pair – bond pair

There are two ways to describe the geometry of a molecule:

- **Electron-Group Geometry** – distribution of electron groups (predicted by VSEPR)
  -could say "electron pairs" but "groups" includes multiple bonds
  -text says "regions of high electron density"
- **Molecular Geometry** – distribution of atomic nuclei
  -the actual shape of the molecule

Representations

Name/Molecular Formula:	ammonia/NH_3	Water/H_2O
Lewis Structure:		
3D Structure:		
Dashed-wedged line structure:	 	 
Molecular Geometry:	trigonal pyramidal	bent or V-shaped
Electron Group Geometry:	tetrahedral	tetrahedral
VSEPR Notation:	AX_3E	AX_2E_2

A=central atom
X=bond to atom
E=electron lone pair

Applying VSEPR Theory

Focus on pairs of electrons in the valence electron shell of a central atom in a structure.

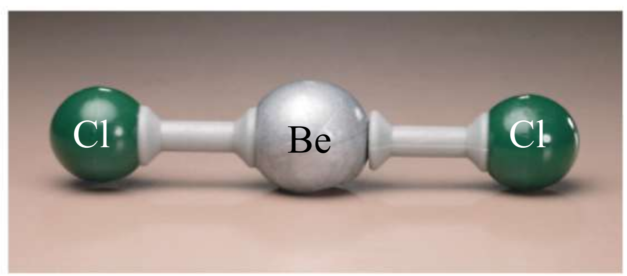
1. Draw a plausible Lewis structure.
2. Determine the number of electron groups around the <u>central atom</u> and identify them as *bond* pairs (X) or *lone* pairs (E).
3. Establish the electron group geometry (both X and E).
4. Determine the molecular geometry (only consider X).

Example

Note: another example of incomplete octet. If we made double bonds to fill octet then we would have a Be^{2-} next to two Cl^{+}, so formal charge wins over octet (like BF_3)

What is the molecular structure of $BeCl_2$?

1. Draw a plausible Lewis structure.
2. Determine the number of electron groups around the central atom and identify them as *bond* pairs (X) or *lone* pairs (E). **AX_2**
3. Establish the electron group geometry (both X and E). **linear**
4. Determine the molecular geometry (only consider X). **linear**

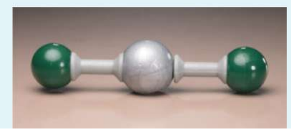


Possibilities for Electron-Group Geometry

2 electron groups	**AX_2**	**linear**
3 electron groups	**AX_3** **AX_2E**	**trigonal planar**
4 electron groups	**AX_4** **AX_3E** **AX_2E_2**	**tetrahedral**
5 electron groups	**AX_5** **AX_4E** **AX_3E_2** **AX_2E_3**	**trigonal bipyramidal**
6 electron groups	**AX_6** **AX_5E** **AX_4E_2**	**octahedral**

Electron-Group Geometry & Molecular Geometry

TABLE 10.1 Molecular Geometry as a Function of Electron-Group Geometry

Number of Electron Groups	Electron-Group Geometry	Number of Lone Pairs	VSEPR Notation	Molecular Geometry	Ideal Bond Angles	Example	
2	linear	0	AX_2	 (linear)	180°	$BeCl_2$	

No other potential molecular geometries

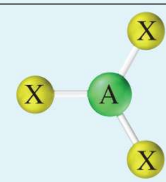
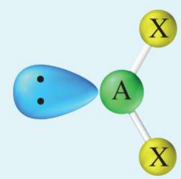
In VSEPR Notation:

- A=central atom
- X=bond and terminal atom
- E=electron lone pair

The molecular geometry is the same as the electron-group geometry <u>only</u> when <u>all</u> electron groups are bond pairs.

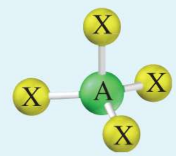
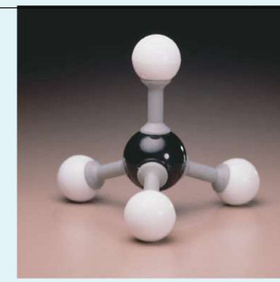
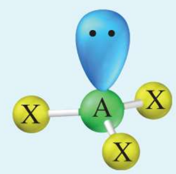
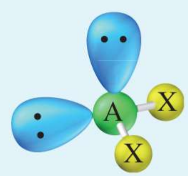
Electron-Group Geometry & Molecular Geometry

TABLE 10.1 Molecular Geometry as a Function of Electron-Group Geometry

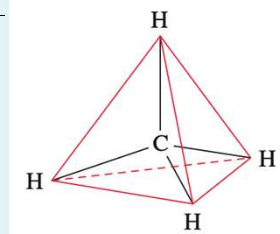
Number of Electron Groups	Electron-Group Geometry	Number of Lone Pairs	VSEPR Notation	Molecular Geometry	Ideal Bond Angles	Example	
3	trigonal planar	0	AX_3	 (trigonal planar)	120°	BF_3	Carey B. Van Loon  Carey B. Van Loon
	trigonal planar	1	AX_2E	 (bent)	120°	SO_2[a]	

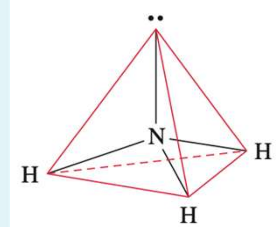
Electron-Group Geometry & Molecular Geometry

TABLE 10.1 Molecular Geometry as a Function of Electron-Group Geometry

Number of Electron Groups	Electron-Group Geometry	Number of Lone Pairs	VSEPR Notation	Molecular Geometry	Ideal Bond Angles	Example	
4	tetrahedral	0	AX_4	 (tetrahedral)	109.5°	CH_4	 Carey B. Van Loon
	tetrahedral	1	AX_3E	 (trigonal pyramidal)	109.5°	NH_3	
	tetrahedral	2	AX_2E_2	 (bent)	109.5°	OH_2	

Are the bond angles the same?





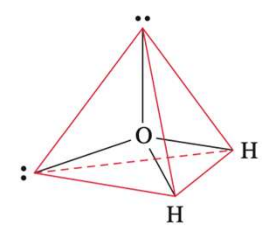
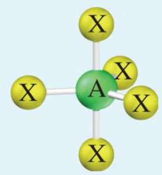
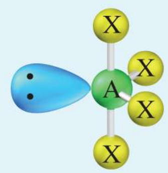
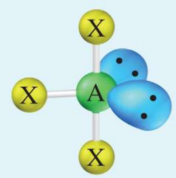
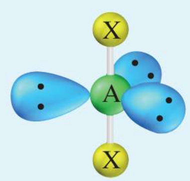
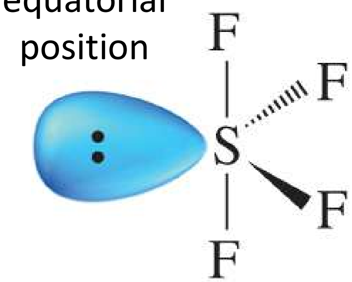


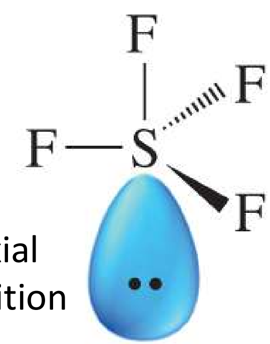
TABLE 10.1 Molecular Geometry as a Function of Electron-Group Geometry

Number of Electron Groups	Electron-Group Geometry	Number of Lone Pairs	VSEPR Notation	Molecular Geometry	Ideal Bond Angles	Example
5	trigonal bipyramidal	0	AX_5	 (trigonal bipyramidal)	90°, 120°	PCl_5  Carey B. Van Loon
	trigonal bipyramidal	1	AX_4E^b	 (seesaw)	90°, 120°	SF_4
	trigonal bipyramidal	2	AX_3E_2	 (T-shaped)	90°	ClF_3
	trigonal bipyramidal	3	AX_2E_3	 (linear)	180°	XeF_2

equatorial position

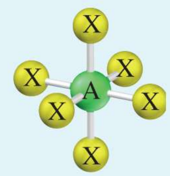
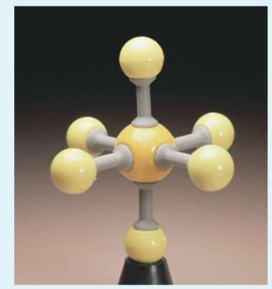
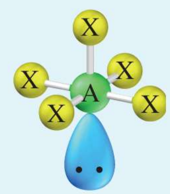
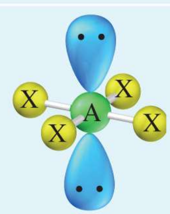


Which lone pair position is correct?



axial position

TABLE 10.1 Molecular Geometry as a Function of Electron-Group Geometry

Number of Electron Groups	Electron-Group Geometry	Number of Lone Pairs	VSEPR Notation	Molecular Geometry	Ideal Bond Angles	Example	
6	octahedral	0	AX_6	 (octahedral)	90°	SF_6	 Carey B. Van Loon
	octahedral	1	AX_5E	 (square pyramidal)	90°	BrF_5	
	octahedral	2	AX_4E_2	 (square planar)	90°	XeF_4	