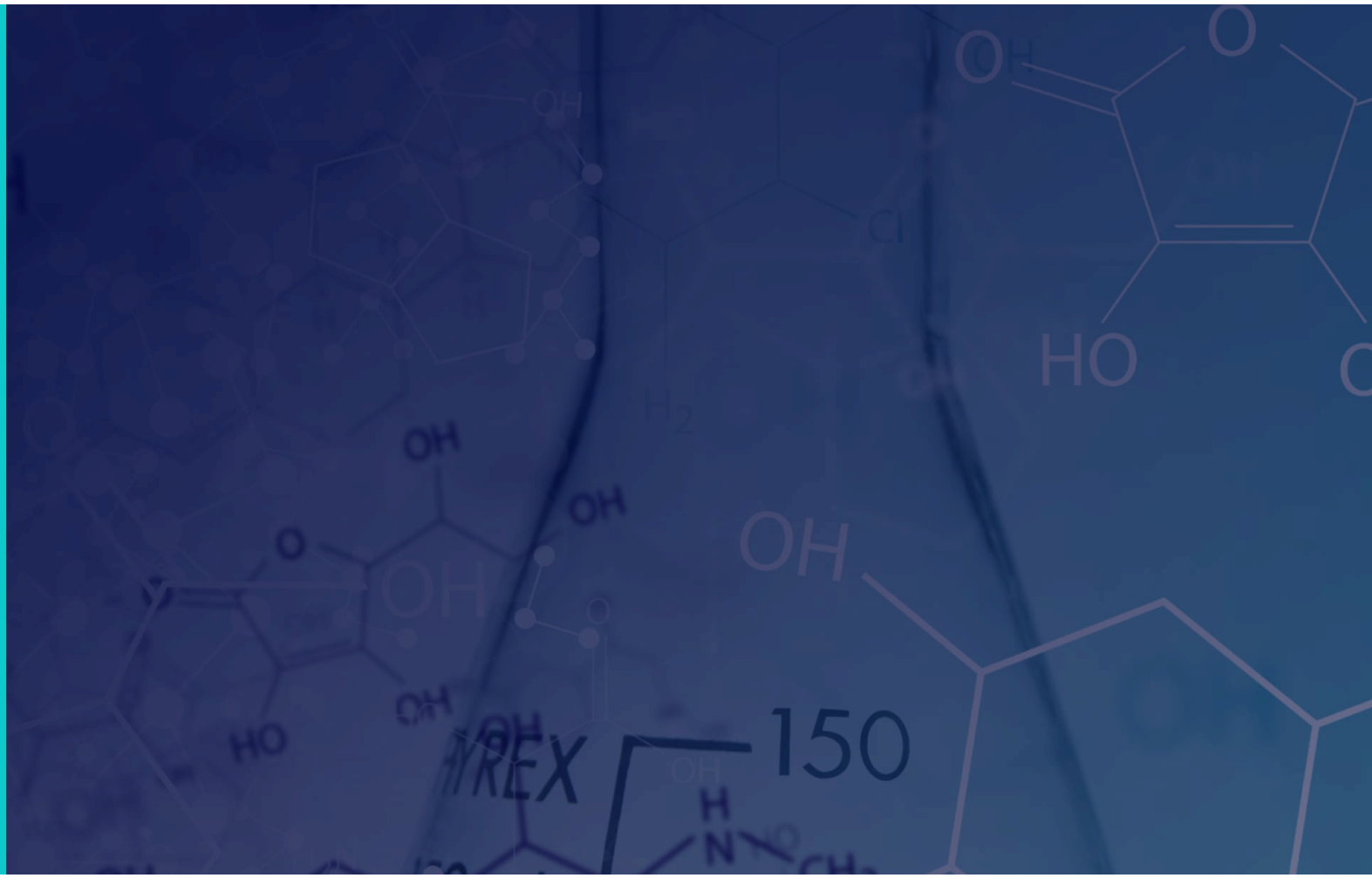

McGill

CHEM 110

Fall 2024, Chapter 4 Notes

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4. The Shapes of Molecules

4.1 VSEPR (Molecular Shapes)

4.1.1

VSEPR Theory

VSEPR aka Valence Shell Electron Pair Repulsion theory: states that repulsion of electron pairs (both bonds and lone pairs) in the valence shell will dictate the molecular geometry of a compound.

Lewis Structure

VSEPR tells us the molecular shape: Square Based Pyramid

Electron Geometry (aka Orbital Geometry or Parent Shape)

Electron geometry is based on the number of **electron groups** around the central atom

$$\boxed{EGs = \text{number of lone pairs of electrons} + \text{number of bound atoms}}$$

EGs are **electron groups**

Example:
How many electron groups does the C atom on the left have?

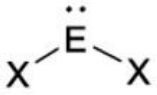
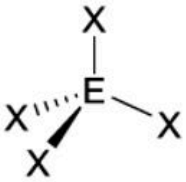
WATCH OUT!

The **triple bond has no effect on EGs** because we are counting the number of bound atoms, so whether there is a **C bound to another C with a single bond, double bond, or triple bond, those will all just count as 1 EG!**

Molecular Shape

The shape of a molecule is determined by where the atoms are located.

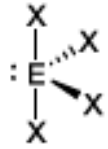
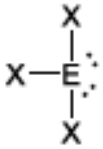
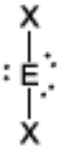
Write the number of electron groups on the left side of the table.

l.p.	b.a.	Parent Shape	Molecular Shape	Picture	Angles
0	2	Linear	Linear	X—E—X	180°
0	3	Trigonal Planar	Trigonal Planar		120°
1	2		Bent		< 120°
0	4	Tetrahedral	Tetrahedral		109.5°
1	3		Trigonal Pyramidal		107°
2	2		Bent		104°

WIZE TIP

The tables in this lesson are very commonly tested on!
Take a few minutes to memorize these tables as you will likely see many questions relating to VSEPR theory on your exams!

Write the number of electron groups on the left side of the table.

l.p.	b.a.	Parent Shape	Molecular Shape	Picture	Angles
0	5	Trigonal Bipyriamidal	Trigonal Bipyriamidal		120^{o}_{eq} 90^{o}_{ax}
1	4		See Saw		120^{o}_{eq} 90^{o}_{ax}
2	3		T-shaped		90^{o}
3	2		Linear		180^{o}
0	6	Octahedral	Octahedral		90^{o}
1	5		Square Based Pyramid		90^{o}
2	4		Square Planar		90^{o}
0	7	Pentagonal Byprimdal	Pentagonal Byprimdal		72^{o}_{eq} 90^{o}_{ax}

Note:

- Wedges mean the bond is coming out of the page and dashes mean the bond is going back into the page.
- LP=lone pairs of electrons
- BA=bound atoms
- **Lone pairs give more push** (are even more repelled by other electrons), which is why wee see the bond angles change slightly.

4.1.2

Example: Parent and Molecular Shape

Determine the parent shape and molecular shape for the following.

a) NH_3

b) SCl_2

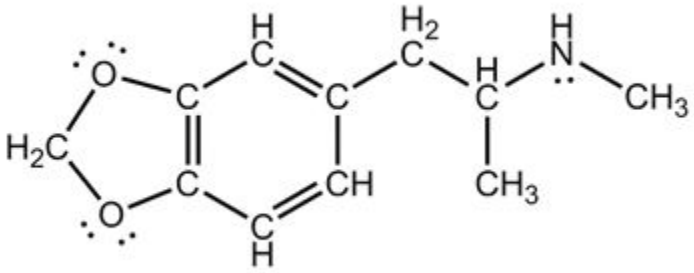
c) IF_7

d) SF_4

4.1.3

Example: VSEPR and Molly

MDMA (3,4-methylenedioxy-methamphetamine) or “Molly” is a psychoactive drug commonly used for recreational purposes, which has been investigated as a treatment for PTSD. It functions by triggering serotonin release and inhibiting serotonin reuptake in the human brain, causing euphoric and empathogenic effects on the user. The structure of MDMA is shown below.



a) What is the molecular shape of the nitrogen atom in MDMA?

b) Approximate the O-C-O bond angle in MDMA?

c) How many atoms with a trigonal planar electron geometry are there in MDMA?

4.1.4

Practice: VSEPR Shapes

Consider the VSEPR for the “best” Lewis diagrams for the following species and use them to answer the next three questions

1. PH_3

2. AlH_4^-

3. IO_3^-

Part 1

Which of the following has a central atom with a tetrahedral electron-pair geometry?

- PH_3 and AlH_4^-
- AlH_4^-
- IO_3^-
- AlH_4^- and IO_3^-
- All of the chemical species have a central atom with a tetrahedral electron pair geometry

Practice: VSEPR Shapes

Consider the VSEPR for the “best” Lewis diagrams for the following species and use them to answer the next three questions

1. PH_3

2. AlH_4^-

3. IO_3^-

Part 2

Which of the following has a trigonal planar molecular shape around the central atom?

- PH_3
- AlH_4^-
- IO_3^-
- None of the above
- All of the above

Practice: VSEPR Shapes

Consider the VSEPR for the “best” Lewis diagrams for the following species and use them to answer the next three questions

1. PH_3

2. AlH_4^-

3. IO_3^-

Part 3

Which of the following displays resonance?

- PH_3
- AlH_4^-
- IO_3^-
- None of the above
- All of the above

4.1.5

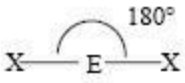
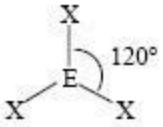
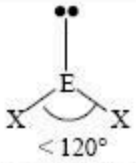
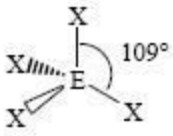
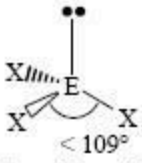
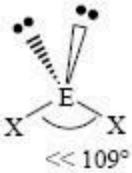
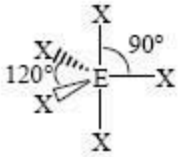
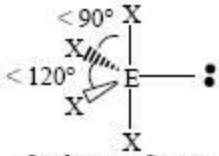
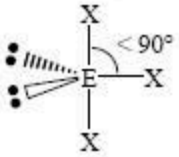
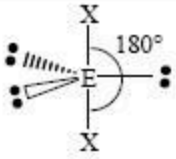
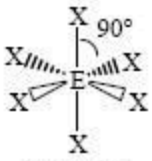
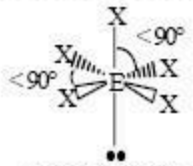
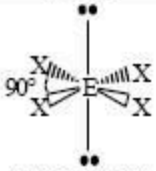
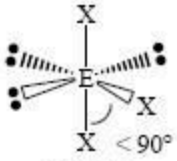
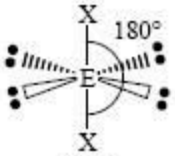
Practice: Bond Angle Identification

Which of the following compounds has a 120^{o} bond angle?

- NH_3
- H_2O
- BF_3
- BrF_5
- SF_6

4.1.6

VSEPR and Molecular Shapes - Cheatsheet

VSEPR Geometries					
Steric No.	Basic Geometry 0 lone pair	1 lone pair	2 lone pairs	3 lone pairs	4 lone pairs
2	 Linear				
3	 Trigonal Planar	 Bent or Angular			
4	 Tetrahedral	 Trigonal Pyramid	 Bent or Angular		
5	 Trigonal Bipyramid	 Sawhorse or Seesaw	 T-shape	 Linear	
6	 Octahedral	 Square Pyramid	 Square Planar	 T-shape	 Linear

The last shape when 7 atoms are bound to the central atom: pentagonal bipyramidal

4.2 VSEPR for Organic Compounds

4.2.1

VSEPR Theory for Organic Compounds

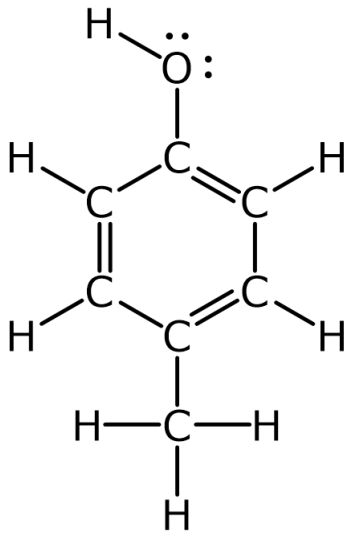
- VSEPR theory doesn't change for organic compounds. Just like for organic compounds with Lewis structures, nothing changes in determining the VSEPR/molecular shape, the only difference is now there are multiple central atoms in the molecule (either C, N, or O, typically), and so each of these central atoms will have a VSEPR/molecular shape.

Ex) $NH_2CH_2CH_2COO^-$

4.2.2

VSEPR Theory of Organic Compounds - Example Problem

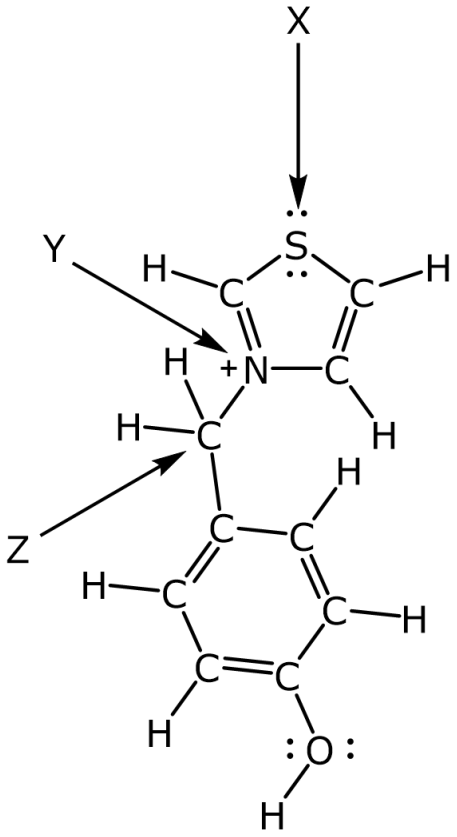
Ex) For the compound: p-hydroxytoluene (shown below), describe the VSEPR shape (aka electron geometry) and molecular shape for each carbon and oxygen atom.



4.2.3

Practice Question: VSEPR Theory for Organic Compounds

Answer the following questions based on the organic structure below.



What is the VSEPR shape (or electron geometry) of atom X?

What is the molecular shape of atom X?

What is the VSEPR shape (or electron geometry) of atom Y?

What is the molecular shape of atom Y?

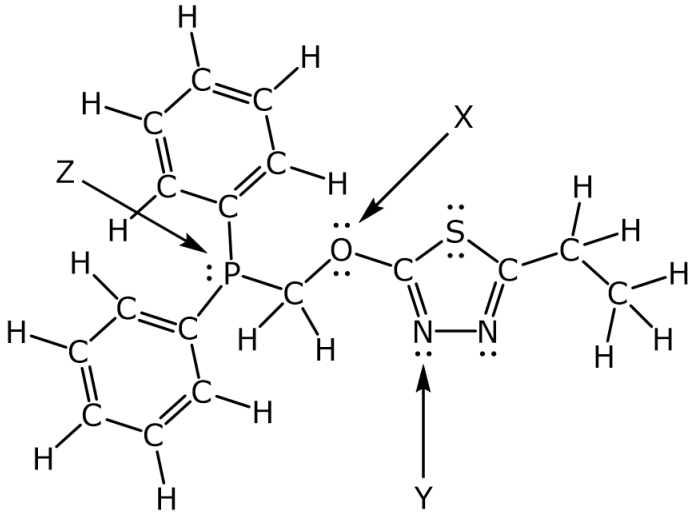
What is the VSEPR shape (or electron geometry) of atom Z?

What is the molecular shape of atom Z?

4.2.4

Practice Question 2: VSEPR Theory for Organic Compounds

Answer the following questions based on the organic structure below.



What is the VSEPR shape (or electron geometry) of atom X?

What is the molecular shape of atom X?

What is the VSEPR shape (or electron geometry) of atom Y?

What is the molecular shape of atom Y?

What is the VSEPR shape (or electron geometry) of atom Z?

What is the molecular shape of atom Z?

4.3 Molecular Polarity

4.3.1

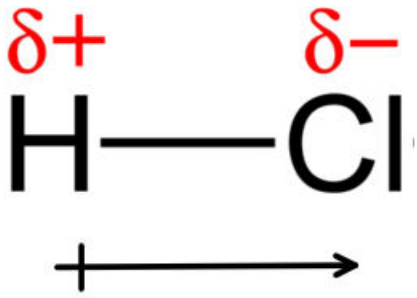
Polar Covalent Bonds

Polar Covalent Bonds:

- Electrons are shared **unequally** between **2 different non-metals**
- There is a difference in EN, $0.4 < \Delta EN < 1.7$

Since electrons are shared unequally in this bond, we say that there is a "**dipole moment**"

- The dipole moment is a vector with both magnitude and direction (more on this later!)
  - Partial negative charge (**δ-**) is assigned to the atom with the **higher EN**
  - Partial positive charge (**δ+**) is assigned to the atom with the **lower EN**
- **The greater the difference in electron density (EN), the greater the dipole moment!**



WIZE TIP

You can think of the dipole moment as a tug of war. The dipole moment (arrow) points towards the winner that is able to pull electrons more towards itself (is more electronegative!)

4.3.2

Molecular Polarity

How can we figure out if a molecule is polar or not?

Recall we talked about **polar covalent bonds** earlier, where **electrons are shared unequally between 2 elements**.

To figure out if a *molecule* is polar, we need to consider all of the bonds and use our knowledge of VSEPR.

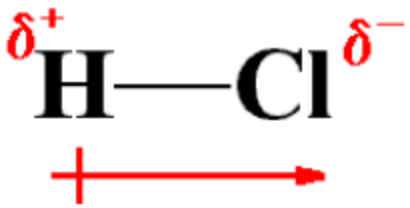
WIZE CONCEPT

If there are **no polar bonds** in the molecule-> it is **non-polar!**

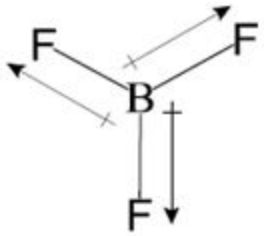
If they are **polar bonds but they are symmetrical**, their dipole moments will cancel each other out-> molecule is **non-polar!**

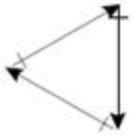
If there are **polar bonds that are not symmetrical**, the dipole moments don't cancel each other out and we are left with a **net dipole moment**-> molecule is **polar**!

Example: Polar Molecule



Example: Non-Polar Molecule





Non-Polar

Example #1: $AlCl_3$

Are there polar bonds? _____

Is there an overall dipole moment? _____

Therefore, $AlCl_3$ is (polar/non-polar): _____

WIZE TIP

In order for a **MOLECULE to be considered polar**, then there must be a **net dipole moment** and the dipoles can't all cross out!

Example #2: Is H_2O a polar molecule?

Are there polar bonds? _____

Is there an overall dipole moment? _____

Therefore, H_2O is (polar/nonpolar): _____

Example #3: Is NH_3 polar or non-polar?

Are there polar bonds? _____

Is there an overall dipole moment? _____

Therefore, NH_3 is (polar/nonpolar) : _____

Example: Net Dipole Moment

Determine whether the following molecules have a net dipole moment (polar molecules). For the ones that do, draw the direction of the net dipole moment.

a) XeF_4

b) CCl_4

c) $CHCl_3$

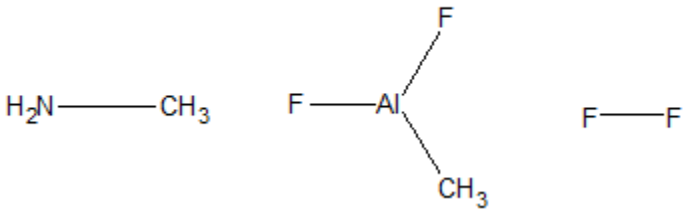
d) SCl_2

4.3.4

Practice: Polar Molecules

Which of the following are polar? (Select all that apply) and indicate the direction of polarity.

A) **B)** **C)**



- [ ] A)
- [ ] B)
- [ ] C)
- [ ] None of the above

4.3.5

Practice: Polar vs Non-Polar

Are the following compounds polar or non-polar?

Part 1

PF_5

- A) Polar molecule
- B) Non-polar molecule
- C) Is a mix of both polar and non-polar bonds so we cannot choose either.

Practice: Polar vs Non-Polar

Are the following compounds polar or non-polar?

Part 2

SF_4

- A) Polar molecule
- B) Non-polar molecule
- C) Is a mix of both polar and non-polar bonds so we cannot choose either

Practice: Polar vs Non-Polar

Are the following compounds polar or non-polar?

Part 3

CF_4

A) Polar molecule

B) Non-polar molecule

C) Is a mix of both polar and non-polar bonds so we cannot choose either