

EXPERIMENT 4 - Molecular Models

Purpose: The purpose of this experiment is to make models of some simple molecules in order to determine the **3-D shape** of molecules.

Using molecular models: The **3-D structure** of molecules greatly influences their chemistry, but this structure is very difficult to show on a 2-D blackboard. Structures drawn on a blackboard only show which atoms are attached together, not what the actual bond angles are. We will use a very simple set of ball and stick models for this experiment.

The following code exists for the bonds:

Bond type	Picture	Model
single bond	—	1 stick
double bond	==	2 sticks
triple bond	≡	3 sticks

There is also a color code for the atoms:

black	==>	carbon
yellow	==>	hydrogen
green	==>	chlorine
red	==>	oxygen
blue	==>	nitrogen

Theory of Valence shell electron pair repulsion theory (VSEPR)

1. **VSEPR** is used to understand **molecular geometry**
2. **Electrons tend to repel one another**, therefore, the **electron “domains”** around an atom will be **as far away as possible** from **other electron domains** around the atom
3. An **electron domain** may consist of
 - a. **a lone pair of electrons**
 - b. **a single bond**
 - b. **double bond**
 - d. **a triple bond**
4. The **number of electron domains** govern the type of **electron pair geometry** and **molecular geometry** that a molecule has

Electron Pair Geometries and Molecular Geometry

<u>Molecule</u>	<u># of e- domains</u>	<u>Electron Domain Geometry</u> (and angle between e- domains)	<u>Molecular Geometry</u>
AB ₂	2	Linear (180°)	Linear
AB ₃	3	Trigonal Planar (120°)	Trigonal Planar (3 bonds)
AB ₂ E	3	Trigonal Planar (120°)	Bent (2 bonds, 1 lone pair); <120°
AB ₄	4	Tetrahedral (109.5)	Tetrahedral (4 bonds)
AB ₃ E	4	Tetrahedral (109.5)	Triangular Pyramidal (3 bonds, 1 lone pair); <109.5°
AB ₂ E ₂	4	Tetrahedral (109.5)	Bent (2 bonds, 2 lone pairs); <109.5°

A = Central Atom

B = Bonded Atom

E = Electron Pair

NOTE: Lone pairs take up more space than electrons that are participating in bonds.

Therefore, for molecules that have lone pairs on the center atom, the predicted bond angles between the atoms involved in the bonds will be somewhat smaller than what is predicted by the electron domain geometries.

I. Structures of simple molecules

A. Carbon dioxide

1. Draw a **Lewis Structure** for carbon dioxide:
2. What **electron domain geometry** does carbon dioxide have?
3. What **molecular geometry** does carbon dioxide have?
4. What **bond angle** around carbon is predicted by VSEPR?
5. Make a **model** of carbon dioxide.
6. Do all **three** atoms lie (approximately) in a **straight line**?

B. Formaldehyde (CH₂O -The carbon is in the middle with the other three atoms around it.)

1. Draw a **Lewis Structure** for formaldehyde.
2. What **electron domain geometry** does formaldehyde have?
3. What **molecular geometry** does formaldehyde have?
4. What **bond angle** around carbon is predicted by VSEPR?
5. Make a **model** of formaldehyde.
6. Do all **three** atoms lie in the **same plane** (or at least close to the same plane)?

C. Ozone

1. Draw a **Lewis Structure** for ozone:
2. What **electron domain geometry** does ozone have?
3. What **molecular geometry** does ozone have?
4. What **bond angle** around the center Oxygen is predicted by VSEPR?
5. Make a **model** of ozone using the black atoms
6. Does the model of ozone that you made look like its molecular geometry?

D. Methane

1. Draw a **Lewis Structure** for a molecule of methane.
2. What **electron domain geometry** does methane have?
3. What **molecular geometry** does methane have?
4. What is the **H-C-H bond angle** that is predicted by VSEPR?
5. Make a **model** of methane.
6. Do any of the **H-C-H bonds** lie in a **straight line**?

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NOTE: At this point you will begin making models that contain nitrogen atoms. Use the blue atom to represent nitrogen. These atoms have 4 or 5 holes in them. The hole on the top (furthest away from the other holes) is where the electron pair should be. **!!!! If there is a hole directly opposite the top hole, this should not be used for bonds or for lone pairs!!!!**

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E. **Ammonia** NH_3

1. Draw a **Lewis Structure** for a molecule of ammonia.
2. What **electron domain geometry** does ammonia have?
3. What **molecular geometry** does ammonia have?
4. What is the **bond angle** around **Nitrogen** that is predicted by VSEPR?
5. Make a **model** of molecule of ammonia.
6. Do you see the **pyramids**?

F. **Water**

1. Draw a **Lewis Structure** for a molecule of water.
2. What **electron domain geometry** does water have?
3. What **molecular geometry** does water have?
4. What is the **bond angle** that is predicted by VSEPR?
5. Make a **model** of water
6. What **other molecule** that we looked at today has the **same molecular shape** as water?
7. Do these two molecules have the **same bond angles**? **Why or Why not?**

G. Hydrogen peroxide (HOOH)

1. Draw a **Lewis Structure** for a hydrogen peroxide molecule. (The order of the atoms is shown above.)
2. What are the **bond angles** around the **oxygen atoms** in hydrogen peroxide?
3. According to VSEPR, should any **three bonded atoms** lie in a **straight line**?
4. Make a **model** of a hydrogen peroxide molecule.
5. Do any **three** of the atoms lie in a **straight line** in the model?

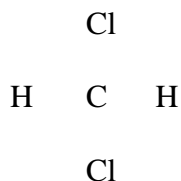
H. Hydrogen cyanide HCN

1. Draw a **Lewis Structure** for a molecule of hydrogen cyanide:
2. Make a **model** of molecule of hydrogen cyanide.
3. Do all **three** atoms lie in approximately a **straight line**?

II. Some more complicated molecules

A. Methylene Chloride (CH₂Cl₂)

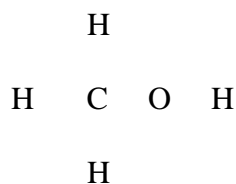
1. Draw the **Lewis Structure** for methylene chloride. The atoms are arranged as shown below



2. Using VSEPR theory, **predict the Cl-C-Cl angle**.
3. Does VSEPR theory predict that the two chlorine atoms and the carbon atom lie in a **straight line**?
4. Make a model of methylene chloride.
5. Does your **model show** the two chlorine atoms and the carbon atom lying in a **straight line**?

B. Methyl Alcohol CH₃OH

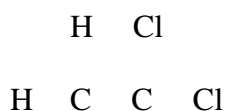
1. Draw a **Lewis Structure** for a methyl alcohol molecule. The atoms are arranged as shown below:



2. Using VSEPR theory, what will be the **bond angle** a) around **carbon**?
b) around **oxygen**?
3. According to VSEPR theory, should **any three of** the atoms lie in a **straight line**?
4. Make a model of methyl alcohol.
5. Is the **prediction** from VSEPR theory (in part 3) **correct**?

C. Dichloroethylene

1. Draw the **Lewis Structure** for dichloroethylene. The atoms are arranged as shown below: (**there is no bond between H and Cl!**)



2. According to VSEPR theory, what are the **bond angles** around the **carbon** atoms?
3. According to VSEPR theory, should the **two hydrogen** atoms and the **two carbon** atoms lie in the **same plane**?
4. According to VSEPR theory, should the **two chlorine** atoms and the **two carbon** atoms lie in the **same plane**?
5. Make a **model** of dichloroethylene.
5. Do **all** the atoms lie in the **same plane**? I.E. is the **entire molecule planar** (flat)?

D. **Acetylene C₂H₂**

1. Draw the **Lewis Structure** for acetylene.



2. According to VSEPR theory, what will be the **bond angles** around both of the **carbon** atoms?
3. Does VSEPR theory predict that **all** of the atoms will lie in a **straight line**?
4. Make a **model** of acetylene.
5. Do **all** of the atoms in the model lie in (approximately) a **straight line**?

E. **H₂CNOH**

1. Draw a **Lewis Structure** for the molecule. The atoms are arranged as shown below:



2. According to VSEPR theory, what will be the **bond angles**:
 - a. around **carbon**?
 - b. around **nitrogen**?
 - c. around **oxygen**?