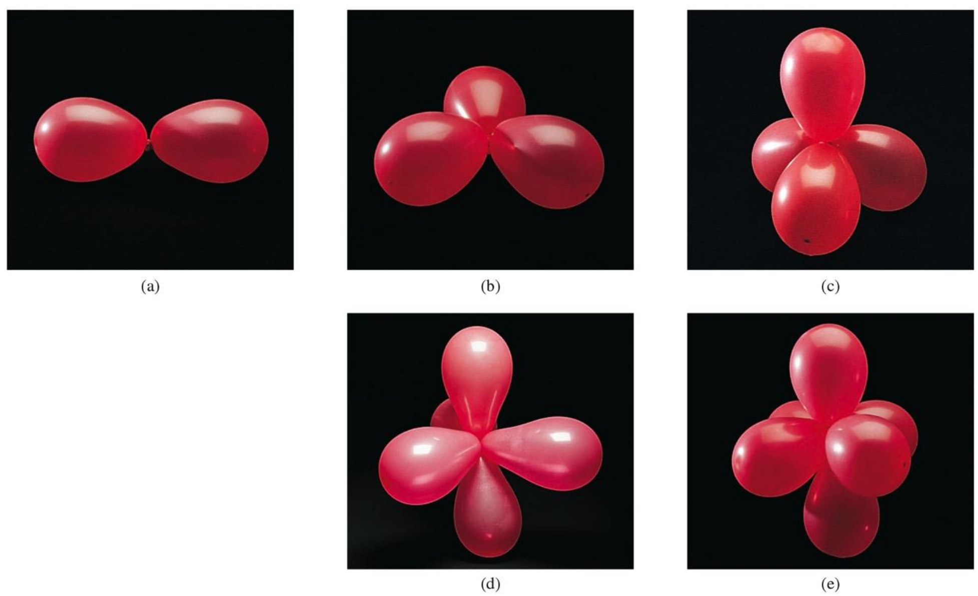
CHEMISTRY 130/170

General Chemistry Lab

Molecular Geometry: The *Shapes* of Molecules



The shapes of molecules, represented here by balloons, provide important information about the chemical and physical properties of that molecule.

DEPARTMENT OF CHEMISTRY

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Introduction

As we have been discussing in class, the electrons of atoms are important in understanding the chemistry of an element. Electron configurations and orbital diagrams can be used to show where the electrons are arranged within an atom. You have also learned that the *core electrons* are located in the lower energy levels and closer to the nucleus, and the *valence electrons* are located in upper energy levels and further from the nucleus. Lewis symbols are used to show the number of valence electrons an element has. It is these valence electrons that are important in **covalent bonding** between atoms in molecules. In this type of bonding two atoms *share* valence electrons to achieve a noble gas electron configuration or an **octet**. The electrons that are shared are called a ***bonded pair*** or bonding electrons and can be represented by two dots (or a line) between the atoms. The other electrons that make up the octet are not shared and are positioned around the atoms as pairs of dots or ***lone pairs*** of electrons. Both types of valence electrons, bonded pairs and lone pairs, are represented by **Lewis structures** and are important for determining the shapes of molecules.

In this lab, you will begin to explore how the *shapes of molecules* are influenced by the number of bonded electron pairs and lone electron pairs around different atoms. The shape of a molecule is important for a variety of reasons. The melting point, boiling point, density, and reactivity of a molecule are all influenced by its shape. There are a number of ways to determine the shape of molecules. *Experimentally*, the structure of a molecule can be determined by spectroscopy and crystallography methods. *Computationally*, you can calculate the geometry of the molecule and the bond lengths and bond angles of the minimum energy structure by solving the Schrödinger equation. However, there are also simple tools available that allow one to quickly predict the approximate geometry of the molecules once an appropriate Lewis structure has been drawn using the valence electrons. The number of bonded pairs and lone pairs of electrons that each atom has is determined from the Lewis structure and the arrangement of these electrons around a central atom is predicted using VSEPR (Valence Shell Electron Pair Repulsion) theory devised by Ronald J. Gillespie and Ronald S. Nyholm. The principle behind this theory is that electron pairs within a molecule *repel* each other due to the fact that they are negatively charged (picture trying to push together the same poles of a magnet). In other words, VSEPR theory states that the electron pairs around a central atom will be arranged to be as far apart as possible in order to *minimize repulsive interactions*. The resulting molecular shape or geometry is the one that *maximizes* the distance between the different electron pairs, both the bonded pairs and the lone pairs. In this lab you will first explore VSEPR using balloons to represent electron groups around a central atom. Your observations and drawings will then be used to assign shapes to real molecules.

As stated above, VSEPR theory considers the bonded pairs of electrons (or bonded atoms) as well as the nonbonding or lone pairs of electrons around the central atom. The inclusion of lone pairs of electrons has dramatic consequences for the structure of the molecules and they must be included in the number of electron pairs to be arranged around the atom. It turns out that the nonbonding pairs of electrons change the observed bond angles from the one which puts only the bonding pairs as far apart as possible.

Pre-lab

This laboratory is designed to help you think about molecular geometries and what factors influence the shapes of molecules and interactions between molecules.

***Pre-lab Assignment*:** Please answer the following questions in your lab notebook. This assignment is due at the beginning of lab. You will not be allowed to start the experiment until this assignment has been completed and submitted to your TA.

1) How do lone pairs of electrons influence the structure of molecules?

2) What does VSEPR stand for? In VSEPR theory, what determines the shape of the molecule?

3) Name the following molecules: CO_2, NH_3, CCl_4, BH_3, SF_4, SO_2.

Procedure

Part 1 – Exploring VSEPR using balloons

As explained in the introduction, VSEPR theory is based on the repulsion of electron groups, *bonded* and *lone* pairs, around a central atom of a molecule. We will use balloon models to explore this concept and to make sketches of different molecular shapes. It is useful to think of electrons in *groups*: bonded pairs and lone pairs. As you work through the below steps, remember that *electron groups* will arrange themselves as far apart as possible, due to repulsion of like charges, around a **central atom**.

1. Obtain four white balloons and two black balloons and inflate them to roughly equal size. The white balloons will represent bonded pairs (groups) of electrons and the black balloons will represent lone pairs (groups) of electrons. The place where the balloons connect to each other will represent a central atom.
2. Hold or clip together two white balloons together to symbolize the arrangement of electron pairs around an atom bonded to two additional atoms (bonded groups of electrons). Sketch a picture of the electron pair arrangement, balloons, in Table 1 in your notebook and determine the maximum angle between the groups.
3. Clip one black balloon to the two white balloons and arrange them as far apart as possible. Sketch a picture of the electron pair arrangement, balloons, in Table 1 in your notebook and determine the maximum angle between the groups. Don't forget to indicate the black balloon on your drawing by coloring it in.
4. Add a second black balloon to this same group of balloons, arrange them as far apart as possible and sketch your results (including bond angles) in Table 1.
5. As in step 4, add *another* black balloon, and sketch your results (including bond angles) in Table 1.
6. Repeat steps 2-4 with three white balloons, then with four white balloons. Sketch the arrangements and determine the maximum angle between groups.
7. Repeat steps 2-3 with five white balloons. Sketch the arrangements and determine the maximum angle between groups.
8. Repeat step 2 one last time with six white balloons. Sketch the arrangements and determine the maximum angle between groups.
9. When you are finished with your sketches, please check with your TA and they will give you the next part of the lab.

Molecular Geometry
DATA SHEETS
Copy the following Tables into your Lab Notebook

Table 1: Sketches of balloons and angle determination

# of electron groups connected to central atom	# of bonded pairs (*white balloons*)	# of lone pairs (*black balloons*)	Sketch of electron group arrangement around central atom (and angle between groups)	Electron domain geometry/molecular geometry *(Part 2)*
2	2	0	*Leave a large space between rows for balloon sketches.*	
	2			
	2			
	2			
	3			
	3			
	3			
	4			
	4			
	4			
	5			
	5			
	6			

Table 2: Sketches of molecular shape, and electron domain/molecular geometry determination

Molecule	Total *valence electrons*	Sketch of Molecular Shape	Electron domain geometry/molecular geometry
H_2	2	*Leave a large space between rows for molecule sketches.*	
CH_4	8		
SCl_2			
PBr_5			
ClF_3			
SF_6			
C_3H_6			
C_2H_4			