

Lab Lecture on VSEPR and SPARTAN
Chem 141 Lab
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Q: What is the purpose of this lab?

To learn two methods to study and predict the shapes of molecules. One is a rule based “paper” method called Valence Shell Electron Pair Repulsion (VSEPR) theory, and the other is the use of computers to apply theoretical models to predict the molecular shapes.

Q: What’s the basic idea behind VSEPR theory?

The basic idea is that molecular shapes are fundamentally determined by electron repulsion, and molecules will take on the shapes that allow electrons to achieve the maximum separation.

Q: How does it work?

First you need to do a Lewis structure.

Q: How do you do a Lewis structure?

The first step is to determine which atom is the center. The center atom is always the one which is least electronegative.

Q: And that works for everything?

Ummm, no. Electronegativities aren’t defined for rare gases. If a rare gas is part of your molecule, it will always be the central atom. Also, sometimes hydrogen will be the atom with the smallest electronegativity, but since under normal circumstances hydrogen makes only one bond, it can’t be the central atom.

Q: What do you do next?

Use the following rules:

- 1) Arrange the atoms around the center atom.

- 2) Count all the valence electrons of the atoms. If the species is an ion add one electron for each negative charge, or subtract one electron for each positive charge.
- 3) Make single bonds between the central atom and all other atoms. This means that we put two electrons between them. Subtract the electrons you've used from the total.
- 4) Fill the octet on all remaining **outer** atoms. (Except for hydrogen, which gets two electrons (which I suppose is a duet))
- 5) If there are any remaining electrons put them around the central atom.
- 6) Calculate the formal charges on each atom. The formal charges on each atom should be as close to zero as possible (and should add up to the total charge on the molecule or ion). If the formal charges are not minimized, then minimize them by making multiple bonds by taking an electron pair from one of the outer atoms and placing it between the outer atom and the central atom. (You may have to do this more than once).

Q: Formal charge? What's formal charge?

It's a way of seeing whether an atom has too few, too many or the most natural number of electrons.

Q: How do you figure out the formal charge?

You count the number of electrons the atom has and subtract the group number. When you count the electrons, you count all of the electrons surrounding an atom that are in lone pairs, and $\frac{1}{2}$ of the electrons in its bonds.

Q: Ok, so now we have the Lewis structure, how do we determine the shape?

With VSEPR.

Q: How do we use VSEPR?

The way we use VSEPR is first to do a Lewis structure for the molecule we are interested in. Then we count the total number of bonds and lone pairs that surround the center atom. For this purpose, we count multiple bonds, if any, as one bond, and any unpaired electrons will have the same effect as a lone pair. The number of bonds and lone pairs determines which of the basic structures we will see.

Q: What are the basic structures?

They are linear, trigonal planar, tetrahedral, trigonal bipyramidal, and octahedral.


Q: Are these basic structures the ones we see?

The actual structure we see will be the basic structure if the central atom is surrounded only by bonds, and will be derived from the basic structure if the central atom is surrounded by bonds and lone pairs. There are lots of cases – I'll list them below:

We will identify each case by a number n , where n is the total number of bonds and lone pairs surrounding the central atom.

The simplest case is for $n=2$. The only way that n can equal 2 is for a triatomic molecule with two bonds. The basic structure and actual structure for $n = 2$ are the same, and are both **linear**.

The next cases are for $n = 3$. **For molecules with $n = 3$, the basic structure is trigonal planar.** If all three electron pairs are in bonds, the actual structure will also be trigonal

planar. An example of this is BCl_3 , which has the Lewis structure . We call a molecule like BCl_3 an MX_3 molecule, where M stands for the center atom and the X for outer atoms. The outer atoms are not necessarily all the same element.

The other $n = 3$ case is one where the center atom is surrounded by two bonds and a lone pair. In this case the actual structure is different from the basic structure. This is because the structure is a description of the arrangement of the atoms in the molecule. In this case the lone pair and the two outer atoms are arranged in a trigonal planar structure, but the three atoms, whose positions are the ones we are interested in, are arranged in a bent structure. The bond angle in this case will be slightly less than the 120° we expect for a trigonal planar basic structure, because a lone pair of electrons takes up more space than electrons in a bond. We call this case MX_2E , where the E indicates a lone pair.

The next group is four $n = 4$. We will consider three cases, MX_4 , MX_3E and MX_2E_2 . **The basic structures of all three will be tetrahedral.** For MX_4 the actual structure will be tetrahedral as well. For MX_3E one of the positions is occupied by a pair of electrons, and the structure of the atoms is called a trigonal pyramid. It looks like a tetrahedron, except the center atom is at one of the vertices of the tetrahedron instead of in the center. Again, because the lone pair takes up more space than the bond, the bond angles are somewhat smaller than the 109.5° expected for a normal tetrahedron. For MX_2E_2 , two of the vertices are occupied by electron pairs, so the result is a bent molecule with bond angle slightly less than 109.5° .

Our next case is $n=5$. We will consider 4 cases here, MX_5 , MX_4E , MX_3E_2 , and MX_2E_3 .

The basic structure for all of these cases is the trigonal bipyramid. For the case of MX_5 , the actual structure is the same as the basic structure, the trigonal bipyramid. For MX_4E , one of the positions is taken by a lone pair. Remember that we have two types of positions in a trigonal bipyramid, the axial and equatorial, which are not equivalent. So which gets the lone pair? The answer is that the lone pair will go in the position that gives the greatest distance from the other electrons. If we put it in an equatorial position, it is 120° away from two atoms and 90° away from two atoms. If it is in an axial position it is 90° away from three atoms, so there is more space in an equatorial position, and that's where the lone pair goes. In fact, for MX_3E_2 both electron pairs will go in equatorial positions, and for MX_2E_3 all three electron pairs will go in equatorial positions. The resulting structures are called a see saw for MX_4E , T shaped for MX_3E_2 , and linear for MX_2E_3 . A special case we need to consider is the case of MX_5 where there are two types of outer atoms. In this case the less electronegative atom goes in the equatorial position. If you have a case like MX_4E , with two different types of outer atom, the electron pair goes in the first equatorial position and is joined there by the less electronegative atoms.

This leaves, **$n = 6$, which will have the octahedral basic structure.** The cases here are MX_6 , MX_5E , MX_4E_2 . There are two other possible combinations, MX_3E_3 , and MX_2E_4 but they are never found to occur in nature. MX_6 will simply have an octahedral structure. MX_5E has an electron in any one of the positions and results in a structure called a square pyramid, where four of the atoms are at the vertices of a square and the fifth is directly above the center. For MX_4E_2 it is important for the electron pairs to be as

far apart as possible, so one will go above the plane and one below.

Q: OK, so that's VSEPR. What do we do with Spartan?

We're going to calculate the structures of several molecules, along with their bond lengths, bond angles and dipole moments.

Q: Why is this better than VSEPR?

VSEPR can only give us general shapes. Spartan and other computational chemistry programs can give us numerical predictions of bond angles and bond lengths. VSEPR can predict whether a molecule will be polar or not. Programs like Spartan can calculate a value for the dipole moment.

Q: How does it work?

The features we'll use are based on force fields. Basically it assigns a force field to each atom, and adjusts the position in the way that minimizes the total energy.

Q: How do we use it?

I think it's best if I do a quick demonstration using the first example in your manual.

Q: Any hints?

Remember that for both parts of the assignment, parts are done in lab, and parts are done at home as exercises.

For the VSEPR part, each of you will be assigned a set of 14 molecules for which you are to determine both Lewis structures and shapes. You should do 10 of these in class today, and the remainder for homework. For the VSEPR section you are required to work individually.

For Spartan, each group will work together on a set of four exercises. You should do the first three in lab (if you have enough time), and complete the fourth as homework. If you run out of time before you do the third, that can be homework as well. The Spartan part of the lab is a group activity, and only one report sheet will be turned in for each group.

Q: Since you mentioned the report sheet, what do we have to do for a lab report?

Just report sheets this week. Each of you should turn in your VSEPR sheets for the 14 molecules, and each group should turn in one Spartan exercise sheet.