Chem 1020 Laboratory

Molecular Models: Lewis Structure and VSEPR Theory

Objectives

- To determine the Lewis structure for a molecule
- To determine the electronic and molecular geometries of a molecule
- To visualize the geometry of a molecule by building its model using a molecular modeling kit

Text References

This experiment is closely based on the lecture material. Review sections 12.6 – 12.10 from the textbook (Zumdahl, 6^{th} ed) on the following topics:

Lewis structures, valence electrons, octet rule, bonding pair, lone pair, multiple bonds, resonance structure, VSEPR theory, electron pair arrangement (or electronic geometry), molecular geometry.

Discussion

When nonmetal atoms get together to form substances, they share their valence electrons—resulting in the formation of covalent bond. A molecule is a group of two or more atoms held together by covalent bonds.

1. Lewis structure is commonly used to describe how valence electrons are distributed and what bonds are formed between atoms within a molecule. Lewis structure is a fundamental representation of a molecule, and it reveals its both chemical reactivity and physical properties such as solubility, melting point, and boiling point.

General Guidelines to Draw Lewis Structure

1) Determine the central atom. Usually it is the one that has the least number of valence electrons and thus needs to make the most bonds to achieve the octet configuration. Place other atoms around it. Carbon has only four valence electrons and always likes to be at the center; hydrogen and fluorine, on the other hand, are never central atoms because each can form only one bond.

2) Count the total number of valence electrons from all of the atoms in the molecule. For a polyatomic ion, you also need to take its charge into consideration (see the following example of NO_3^-).

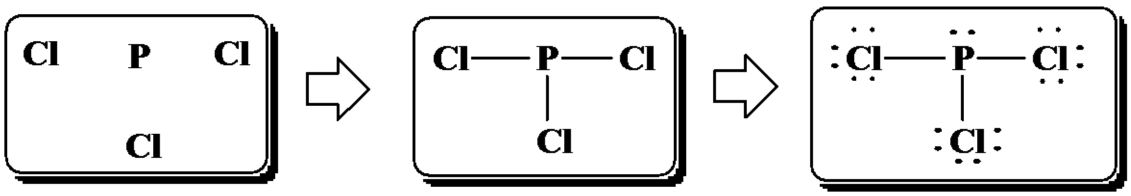
3) Form a single bond (using a pair of electrons) between the central atom and each of the surrounding atoms.

4) Arrange the remaining electrons first on surrounding atoms and then on the central atoms to make sure they have duet (for H) or octet (for all the other elements) configuration.

5) If the central atom isn't left with enough electrons, take a lone pair from one of the surrounding atoms and convert it into a second bond between the central atom and this surrounding atom. They are also called doubled-bonded with each other.

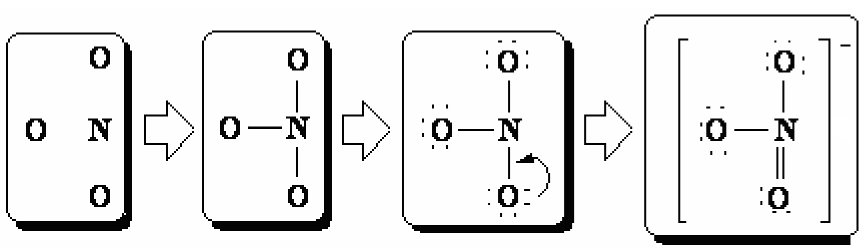
Example: Determine the Lewis structure for PCl_3.

1) Phosphorus has only five valence electrons and each Cl atom has seven. Apparently, P is the central atom and surrounded by three Cl atoms.
2) Total Valence Electrons = $5e^-$ (P) + $3 \times 7e^-$ (3 Cl) = $26e^-$
3) Make single bonds between P and the three Cl atoms, which uses $3 \times 2e^- = 6e^-$
4) The remaining $20e^-$ ($=26e^- - 6e^-$) will be spread on atoms as lone pairs. First on the three surrounding Cl atoms, each of which needs 6 more electrons to get to an octet. So $18e^-$ is needed. The last two electrons are left for the central P atom, which gives it an octet as well. Double-check to make sure every atom has an octet.



Example: Determine the Lewis structure for nitrate ion NO_3^-.

1) Nitrogen has only five valence electrons and each O atom has six. Apparently, N is the central atom and surrounded by three oxygen atoms.
2) Total Valence Electrons = $5e^-$ (N) + $3 \times 6e^-$ (3 O) + $1e^-$ = $24e^-$ (the extra valence electron comes from the -1 charge of the ion)
3) Make single bonds between N and the three O atoms, which uses $3 \times 2e^- = 6e^-$
4) The remaining $18e^-$ ($= 24e^- - 6e^-$) is just enough to be spread evenly on the three surround O atoms as lone pairs to give each an octet.
5) The central N atom still lacks $2e^-$, so bring one of the lone pairs from one of the O atoms and put it in between N and this O to make a second bond.



Consult the lecture textbook for more examples.

2. VSEPR Theory (Valence Shell Electron Pair Repulsion Theory)

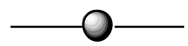
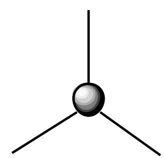
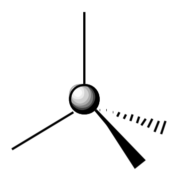
The correct Lewis structure of a molecule provides a basis for determining the shape of this molecule using VSEPR theory. The VSEPR theory recognizes that all electron pairs (including both bonding pairs and lone pairs) are of the same charge and therefore ought to repel one another and position themselves as far apart as possible around the central atom.

Steps to Predict the Molecular Geometry Using VSEPR Theory

1) Draw the correct Lewis structure.

2) Count the total number of electron regions: lone pair regions and bonding pair regions (a double or a triple bond is counted as only one region). *Note: count the regions on the central atom only, and do not include the lone pairs on the surrounding atoms.*

3) Arrange the electron regions in such a way that they are as far apart as possible to minimize repulsion. The resulting geometry is called electronic geometry.

# of Electron Regions	Electronic Geometry	3-D Representation
Two	Linear	
Three	Trigonal planar	
Four	Tetrahedral	

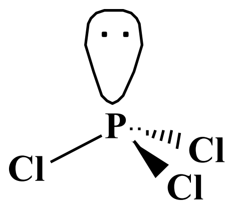
4) Determine the molecular geometry by ignoring the lone pair regions in the above electronic geometry and only looking at the arrangement of the bonding pair regions. Some common geometries are: linear, bent, trigonal planar, tetrahedral, and trigonal pyramid. Please check textbook (Zumdahl 6th ed) Table 12.4 on page 370 for details.

Example Determine the electronic geometry and molecular geometry for PCl_3.

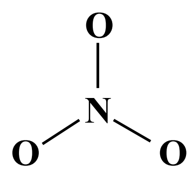
1) The Lewis structure of PCl_3 is determined and shown on page 2.
2) The central P atom has totally four electron regions (coming from one lone pair region and three bonding pair regions).
3) These four electron pairs assume a tetrahedral geometry in order to be as far apart from one another as possible. This is the electronic geometry of PCl_3.
4) Only focus on the arrangement of the P and three Cl atoms in the above electronic geometry. They have a trigonal pyramidal molecular geometry (see the figure on the next page).

Example Determine the electronic geometry and molecular geometry for NO_3^-.

1) The Lewis structure of NO_3^- is determined and shown on page 2.
2) The central N atom has totally three electron regions. Be careful, the double-bond is counted as one region even though it contains two bonding pairs.
3) These three electron regions have to take a trigonal planar geometry to be far apart. This is the electronic geometry of NO_3^-.
4) Only focus on the arrangement of the N and three O atoms in the above electronic geometry. Since there is no lone pair on the N atom, its molecular geometry is exactly the same as its electronic geometry – trigonal planar (see the figure below).



Geometry of PCl_3



Geometry of NO_3^-

Lab Procedure

1. You must bring your lecture textbook to the lab.
2. You will be working individually today in the lab.
3. Obtain a data sheet and a molecular modeling kit from your lab instructor.
4. For each molecular on the data sheet,
   1) write the correct Lewis structure,
   2) build the model of the molecular using the molecular modeling kit,
   3) make a sketch of the electronic geometry, and
   4) determine the electronic geometry and molecular geometry using various geometric names.
4. Organize your molecular modeling kit and return it to your lab instructor.

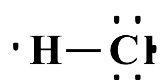
Pre-lab Exercise for Molecular Modeling (Complete before coming to the lab)

1. Count the total number of valence electrons for each of the following molecules and ions.

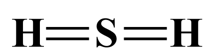
   HCl H_2S ClO_3^- NH_4^+ C_2H_6O

2. Are the following Lewis structures reasonable? Consider the total number of valence electrons, and check if hydrogen atoms have duet and the other atoms have octet valence shell electron configuration. If the structure is not reasonable, explain.

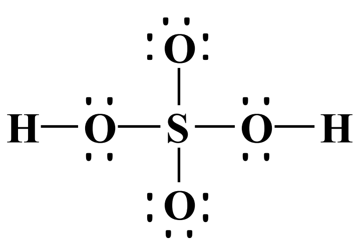
1) HCl



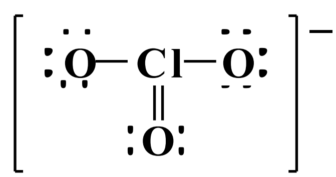
2) H_2S



3) H_2SO_4



4) ClO_3^-



5) C_2H_6O