Protocol | Applications of Molecular Geometry

Lewis Structures, Molecular Geometry, and Polarity

Bring a laptop computer to lab this week.

Download the pdf here. (https://gatech.instructure.com/courses/334258/files/42101221?wrap=1)

Introduction

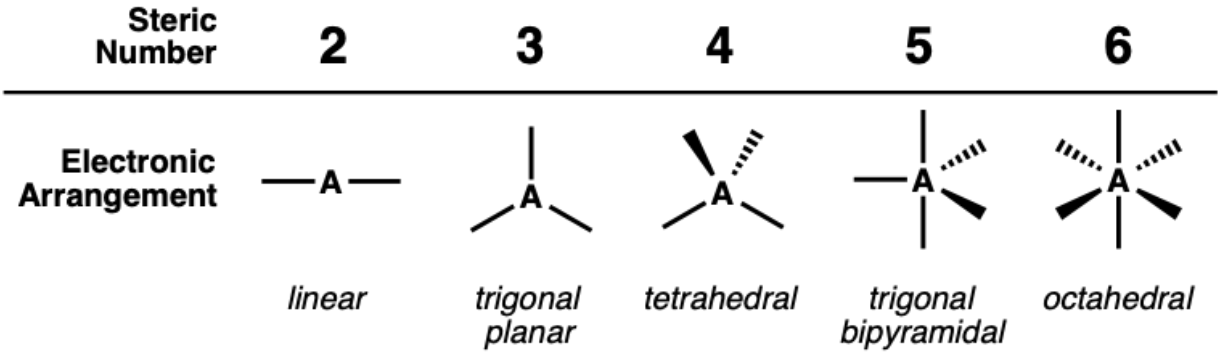
Watch the **introduction and theory video (https://www.youtube.com/watch?v=BcwPOls_qyU&list=PLykBd3LSjfsTuLiqtKlKJdPrRbjfcamGC&index=8)** for this experiment.

Lewis structures are depictions of molecular structure on the microscopic level. They show how electrons are shared between atoms in a molecule and help us understand the structure and reactivity of compounds. To the trained eye, a Lewis structure reveals a wealth of information about how a compound is expected to behave. In this experiment, we will focus on deducing the geometry of groups around an atom within a molecule from the numbers and types of electrons surrounding it. Information about molecular shape can in turn be used to reason about the properties and even the reactivity of the associated compound. For example, whether a molecule is *polar* or *nonpolar* depends on its number and types of atoms as well as its geometry.

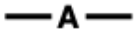
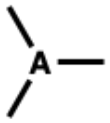
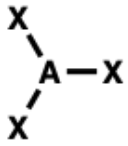
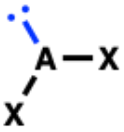
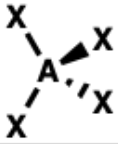
A variety of different approaches have been developed for drawing valid Lewis structures given a molecular formula. They generally focus on first identifying and drawing how the atoms are connected to one another with sigma bonds (usually using the way the formula is written as a guide), then adding valence electrons to satisfy the *octet rule* and minimize charges on the atoms as much as possible. Double and triple bonds, which indicate the sharing of multiple pairs of electrons, appear when two atoms need to share more than two electrons in order to satisfy the octet rule. Core electrons do not appear in Lewis structures because they are not involved in bonding in any important way.

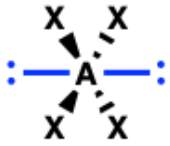
The key to determining molecular geometry from a Lewis structure is to identify the number of valence *electron-pair domains* around the central atom (or multiple central atoms, for larger molecules). An electron-pair domain is defined as a contiguous region of space in which a group of electron pairs are likely to be found. A double or triple bond is associated with a single electron-pair domain because the electron clouds for the sigma and pi bonds overlap. Nonbonding electron pairs (*lone pairs*), which are localized on individual atoms, each occupy a distinct region of space and thus have their own electron-pair domains.

The number of electron-pair domains surrounding a central atom is called the *steric number* of the atom. Because each domain is negatively charged, we expect that the molecular geometry will reflect the idea that the domains are spaced as far apart as possible, to minimize repulsion between negatively charged electrons. This idea is called the *valence shell electron pair repulsion (VSEPR) theory*, and it is the essence of a straightforward method for determining the geometry of a molecule from its Lewis structure. VSEPR theory ignores the exact content of each electron-pair domain and instead assumes that the arrangement of electron-pair domains about an atom is wholly determined by its steric number. Put another way, given the steric number of an atom we can immediately conclude its *electron-group arrangement*, the spatial distribution of electron-pair domains around the atom.



We distinguish between the electron-group arrangement and the *molecular geometry*, the arrangement of bonds and atoms alone. Determining the molecular geometry requires an understanding of both the electron-group arrangement and the number of lone pairs at the central atom. After adding lone pairs to the electron-group arrangement in the appropriate positions, we examine the remaining atoms to determine the molecular geometry. For example, consider the molecule NF_3. The central nitrogen in this molecule bears three single bonds and one lone pair, a total of four electron-pair domains. Hence, its electron-group arrangement is tetrahedral. However, its molecular geometry is *not* tetrahedral because one of its domains contains a nonbonding lone pair. The nitrogen and three fluorine atoms form the shape of a pyramid, so the molecular geometry of NF_3 is *pyramidal* (or *trigonal pyramidal*).

Steric Number	Electron-group Arrangement	Lone Pairs at Central Atom	Shape
2	*linear* 	0	*linear* 
3	*trigonal planar* 	0	*trigonal planar* 
		1	*bent* 
4	*tetrahedral* 	0	*tetrahedral* 
		1	*(trigonal) pyramidal* 
		2	*bent* 
5	*trigonal bipyramidal* 	0	*trigonal bipyramidal* 
		1	*see-saw* 
		2	*T-shaped* 
		3	*linear* 
		0	*octahedral* 

6	*octahedral* 	1	*square pyramidal* 
		2	*square planar* 

Understanding the geometry of a molecule is useful for a number of reasons. Most simply, the molecular geometry gives us information about the spatial situation of the central atom: is it crowded or open? Along what trajectories can reactive molecules approach? In addition, molecular geometry provides insight into the overall distribution of electrons in the molecule. Molecules containing different types of atoms have covalent bonds that are *polarized* toward the more electronegative atom in the bond. Polarization means that the electron density is greater on one atom than the other, and it often results in interesting properties or reactivity. Bonds with a significant degree of polarization are called *polar*, and we represent the polarization of polar bonds using a vector coincident with the bond that points from the positive end of the bond to its negative end (a *bond dipole moment*).

In addition to evaluating the polarity of a bond, we can also evaluate the polarity of a molecule as a whole by asking whether it has a permanently asymmetric distribution of electrons and a nonzero *molecular dipole moment*. The molecular dipole moment is simply the sum of the individual bond dipoles. This is a vector sum, meaning that the geometries of the bonds are important—and this is where the molecular geometry comes in! We must consider the three-dimensional geometry of the bond dipoles to determine whether they cancel one another upon addition or not. Canceling that results in a net dipole moment of zero indicates that the molecule as a whole is nonpolar; when the addition of bond dipoles results in a nonzero molecular dipole moment, we conclude that the molecule as a whole is polar.

Procedures

A. Drawing Lewis Structures

1. In your lab notebook, draw Lewis structures for the following molecules. Include all valence electrons (including nonbonding electrons) in the structures. Leave some space underneath each structure.
   A. CO_2
   B. SF_2
   C. AlF_3
   D. PCl_3
   E. CH_3OH (methanol)
   F. CBr_4

G. CH_2O (formaldehyde)
H. NH_3
I. SF_6

B. Predicting and Observing Molecular Geometry

1. Underneath each Lewis structure that you drew in Part A, predict the *molecular geometry* at the central atom. First, determine the steric number, then the electron-group arrangement, and finally the molecular geometry. For molecule E, treat carbon as the central atom.
2. Visit **this simulation (https://phet.colorado.edu/sims/html/molecule-shapes/latest/molecule-shapes_en.html)** and use the *Model* mode to construct a model of each of the molecules in Part A. Take a screenshot of each model and paste it into an empty document. Ensure that you can associate each molecule with its formula later by typing in the formula above or below each image. Compare the geometries shown in the simulation to your predictions in step 1.

C. Predicting and Observing Molecular Dipole Moment

1. In your lab notebook, draw bond dipole vectors for each of the bonds in CO_2. Discuss with your lab partner to ensure the directions and orientations of your bond dipole vectors are correct. Predict whether the molecule has a net dipole moment.
2. Construct CO_2 in the MolCalc online model kit **here (https://molcalc.org/)**. After building the molecule, click the *Optimize* button to ensure the geometry is correct and then the *Get Properties* button to display various properties of the molecule.
3. Visit the *Polarity and Solvation* tab, click the *Surface* switch to turn off the electrostatic potential surface, and click the *Dipole* switch to display the net dipole derived from vector addition of the bond dipoles. (If the molecule has no net dipole, nothing will be displayed.) On or near the Lewis structure in your lab notebook, draw the net molecular dipole vector; if there is no net dipole, write "zero dipole" under the structure. Grab a screenshot of the structure with the net dipole vector (or no net dipole) displayed and paste it next to your image of the geometry from step B-2.
4. Finally, turn off the *Dipole* switch and turn on the *Surface* switch, which will display the distribution of charge on a surface surrounding the molecule (molecular electrostatic potential or MEP). Negative charge is red, positive charge is blue, and neutral charge is green. Grab a screenshot of the structure with the MEP and paste it next to your image with the molecular dipole vector (or no net dipole).
5. Build the molecule in **this model kit (https://chemagic.org/molecules/amini.html)**, optimize the structure and use the Dipoles button to show the bond dipoles. Grab a screenshot of the molecule with its bond dipoles.
6. Repeat steps C.1 – C.5 for the remaining eight molecules from Part A. Before moving forward, make sure you have a Lewis structure and images of a geometric model, molecular dipole vector (or no net dipole), and MEP for all nine molecules.

7. Examine your molecular dipole vectors and MEPs and determine whether each molecule is polar or nonpolar. Record the results in your lab notebook.

Post-lab Calculations and Data Workup

For the post-lab assignment for this experiment, you will create a solution guide for a problem based on one of the nine molecules investigated. The problem statement is simply "Is *X* a polar or nonpolar molecule?" Choose one of the molecules whose molecular geometry is *not* the same as its electron-group arrangement. Use the Lewis structure in your lab notebook and your images of the geometry, bond dipoles, molecular dipole, and MEP to solve this problem and prepare a detailed solution guide for the problem based on instructions in the post-lab assignment. Your solution guide should be detailed enough that starting *only* from the molecular formula, the reader could rigorously arrive at the correct conclusion about the polarity of the molecule.