Geometry of Molecular Species

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Introduction:
Some time ago you attended the opening of your friend’s art show. You thought to yourself that she is an amazing artist because she uses shapes and lines in such a “natural” way. Sometime later, you are driving by downtown Dallas and suddenly the shapes of the various buildings strike you in a way they had not before. You find your mind wondering about how the different lines and shapes are so visually appealing as you drive home. My goodness! You realize you are becoming more appreciative of the subtle things.

Geometry, or shape, does not only apply to visible structures. Considering the smallest possible particle of covalent (molecular) substances, you will find there is geometry associated with molecules as well. In fact, R.J. Gillespie (1963, 1970) provided a conceptually simple approach to molecular three-dimensional structure of chemical compounds formed from the representative (main group) elements. This approach is called Valence Shell Electron Pair Repulsion Theory (VSEPR).

Lewis Structures
Before we can determine the geometry of a molecule, we first have to draw its Lewis structure. A Lewis structure is a two-dimensional representation of all the atoms in a covalent species and their valence electrons, each represented with a dot. Following are the steps to drawing the Lewis structure for a molecular species.

1. Count the total number of valence electrons in the molecule or ion. For cations make sure you subtract the number of electrons missing that gave rise to the net positive charge. For anions, add the number of electrons gained that gave rise to the net negative charge.
2. Determine the central atom and connect the atoms accordingly. The central atom is:
   a. NEVER hydrogen,
   b. the least electronegative atom, or
   c. the atom needing the most electrons to reach octet.
3. Once the atoms are all connected, count the electrons represented in the bonds. Remember that each covalent bond is two electrons.
4. Subtract the number of electrons in the bonds from the total number of electrons. Place the remaining electrons around the peripheral (non-central) atoms so they reach octet. Remember that H needs only two electrons to reach octet. If there still are more electrons, place them around the central atom.
5. Check to see if all atoms are at octet. If the central atom is not at octet, move one of the lone (nonbonding) pairs from a peripheral atom and make it a bonding pair with the central atom. In this case, you will have an atom that is sharing two pairs of electrons with the central atom. This is called a double bond. If the central atom still hasn’t reached octet, make another lone pair a bonding pair with the central atom. You can have up to three pairs of electrons shared between two atoms, or a triple bond.
6. If you have a species that has an odd number of valence electrons, it is a free radical. It will not have all the electrons paired nor will all atoms fulfill their octet.
7. If you have a species where the central atom has a valence shell of \( n \geq 3 \), it has \( d \)-orbitals available in its valence shell and can accommodate more than 8 electrons. These atoms will often go beyond 8 electrons, as in the case of \( \text{PCl}_5 \). They are said to have an expanded octet.

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The Problem:
You will (1) construct a table of geometries based on models you build, and (2) determine the molecular geometry of common molecules and ions.

Table of Geometries
Obtain a small piece of modeling clay and 6 toothpicks. Begin by working the clay into a smooth sphere. First, insert two (2) toothpicks into the clay so that the outer ends of the toothpicks are as far apart as possible. Draw the structure you created. Focusing on the toothpicks, what shape/geometry do they form? What is the angle between them? Now remove the toothpicks and smooth out the clay. Insert three (3) toothpicks into the clay so that the outside ends of the toothpicks are as far apart as possible. Draw the structure you created. Focusing on the toothpicks, what shape/geometry do they form? What is the angle between them?

Now remove the toothpicks and smooth out the clay. Insert four (4) toothpicks into the clay so that the outside ends of the toothpicks are as far apart as possible. If the structure you make looks like an X, you are not thinking in three-dimensions. Realize that you should use all three dimensions to accomplish this task. Consider having angles greater than 90°. Draw the structure you created. Focusing on the toothpicks, what shape/geometry do they form? Measure the angles between the toothpicks in your model. What are the angles? Are they all fairly equivalent? Keeping the model intact, remove ONE toothpick from the structure you have. What structure remains? How is it different from the structure you had when you started with only three toothpicks? Now remove one more toothpick. What structure remains? How is it different from the structure you had when you started with only two toothpicks?

Remove the toothpicks and smooth out the clay. Insert five (5) toothpicks into the clay so that the outside ends of the toothpicks are as far apart as possible. Draw the structure you created. Focusing on the toothpicks, what shape/geometry do they form? What are the angles between them? Are they equivalent? Now remove ONE toothpick from the structure you have. Can you remove different toothpicks and end up with different structures? If so, which is the most stable? What structure remains? How is it different from the structure you had when you started with only four toothpicks? Now remove one more toothpick. What structure remains? How is it different from the structure you had when you started with only three toothpicks? Remove one more toothpick. What structure remains? How is it different from the structure you had when you started with only two toothpicks?

Remove the toothpicks and smooth out the clay. Insert six (6) toothpicks into the clay so that the outside ends of the toothpicks are as far apart as possible. Draw the structure you created. Focusing on the toothpicks, what shape/geometry do they form? What are the angles between them? Are they equivalent? Now remove ONE toothpick from the structure you have. What structure remains? How is it different from the structure you had when you started with only five toothpicks? Remove a second toothpick. Can you remove different toothpicks and end up with different structures? If so, which is the most stable? What structure remains? How is it different from the structure you had when you started with only four toothpicks?

Molecular Geometry of Common Molecules and Ions
The central atom(s) of a molecule has a certain number of valence shell electron pairs around it, whether bonding or nonbonding. These electron pairs repel each other, and consequently will be as far apart as possible in order to give the most stable arrangement of electron pairs. This is the same concept you used when placing the toothpicks in the clay for the first part of this exercise. Both bonding and nonbonding valence electron pairs occupy space and, thus, help determine the molecular structure. Since we can only detect nuclei (they have detectable mass) and not electron pairs, only the bonding regions around an atom are visible to us.

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To determine the molecular geometry first you must draw a Lewis structure. Focus on the central atom. Determine the number of regions of electron density (zones) around the central atom, both bonding and nonbonding. Consult the table you constructed in the previous section and determine the electron pair (overall) geometry. Now consider how many of the regions are visible (bonding) and determine the “visible” geometry of the molecular species. This is simply called the geometry.

Draw the Lewis structures for the species given in the table. Determine their electron-pair geometry and their (molecular) geometry.

**Critical Data/Discussion to Include in Your Lab Report:**

- Completed tables for parts 1 and 2
- Cite references in the format specified by your instructor

**Works Cited**
