

Dougherty Valley HS AP Chemistry
Molecular Bonding and Structure of Covalent Compounds

Background Information

One of the most important topics in the study of molecules is how they are put together-how their atoms are arranged relative to each other in space. A theory of chemical bonding that explains **molecular shape** is a useful tool for the modern chemist because *the manner in which atoms are bonded together to make a molecule influences the chemical and physical properties of that molecule*. We have learned in class that the water molecule has a “bent” geometry. If the water molecule were linear instead of bent, the chemistry of life as we know it would be different.

The shape of a molecule cannot be easily predicted from its molecular formula. Molecules that have apparently similar molecular formulas do not necessarily have the same molecular shape. Why is it, for example, that a molecule of aluminum chloride (AlCl_3) is planar whereas nitrogen trichloride (NCl_3), a molecule that is similar to AlCl_3 in that it has one central atom and three different atoms bonded to it, is shaped like a pyramid? Similarly, why does CO_2 have a linear geometry, while sulfur dioxide, SO_2 , has a bent geometry? A better understanding of these three-dimensional structures of molecules will give better insight into these questions and will suggest explanations for them.

Refer to your notes for background information about draw Lewis structures and about the VSEPR theory.

Polarity of Molecules

An additional property of molecules that can be explained by their molecular shape is polarity. In many molecules, one end of the molecule has an excess of negative charge while the other end has an excess of positive charge, even though the molecule as a whole is electrically neutral. Molecules with this imbalance of electrical charge are called **polar molecules** and they are said to possess a **dipole moment**. Most such molecules contain **polar bonds**, which are bonds in which electrons are shared unequally by the bonding partners. The atom with the greater ability to attract the electrons pairs is said to have a higher **electronegativity** than the other atom. Several electronegativity scales have been established from experimental data.

Molecules without an imbalance of electrical charge are called **nonpolar** molecules and they may or may not contain polar bonds. Nonpolar molecules have a net zero dipole moment. Molecular polarity is dependent not only on the charge distribution around the individual atoms but also upon the molecular shape. **Homonuclear diatomic** molecules such as Br_2 are necessarily Nonpolar because the bond is between like atoms. Thus, the sharing of electrons between atoms is equal because the electronegativities of the atoms involved in the sharing is equal. **Heteronuclear diatomic molecules** such as HF are almost always polar. That is, the electrons are not shared equally. The more electronegative atom (in this case, fluorine) has the ability to attract electrons in the shared bond to itself and hence has the excess negative charge.

For polyatomic molecules, both of the polarities of the bonds and the orientation of the bonds contribute to the overall polarity of the molecule, as shown in Figure 8-3. The linear CO_2 molecule, for instance, contains two polar covalent bonds, yet is a Nonpolar linear molecule. The polarities of the two bonds are equal, but their charge separations are precisely in opposite directions, resulting in a zero dipole moment. The bent H_2O molecule, on the other hand, is a polar molecule. The two polar bonds are also equal in magnitude, but do not cancel each other.

A molecule having the symmetry of the structures in Figure 8.3 (without nonbonding electron pairs on the central atom such as found in BeCl_2 , CH_4 , PCl_5 , or SF_6) will have a zero net dipole moment because contributions of electron displacement in each bond cancel one another. In general, molecules on which the central atom carries only one nonbonding pair will be polar. For example, the SO_2 molecule described earlier is a polar molecule. Ammonia, NH_3 , has nitrogen atoms at the apex of the pyramid and the hydrogen atoms at the three corners of the bases and is also polar. However, CO_2 , a linear molecule with no non-bonding pairs is non-polar.

Materials

We will be using a Phet Simulation site [HERE](#).

Once at the website, you will click on MODEL and start building

Experimental Procedures

Molecules: CS₂, HCN, SO₃, NO₂⁻, CCl₄, NCl₃, H₂O, TeCl₄, XeF₂, SF₆, XeF₄, SbCl₅²⁻, IOF₅, I₃⁻, ICl₄⁻, AsF₅

For each molecule, do the following — see Building Molecules data table:

1. Draw Lewis Structure
 2. * Determine the following for each atom:
 - a. Number of lone pairs and bond pairs around the central atom.
 - b. AXE formula (A center atom, X bonded atoms, E lone pairs)
 - c. Steric Number
 3. * Using the information from Step 2 and a VSPER chart (which should be memorized!), determine the following:
 - a. Electronic Geometry (*linear, trigonal planar, tetrahedral, trigonal bi-pyramidal, or octahedral*)
 - b. Molecular Geometry (*linear, trigonal planar, trigonal pyramidal, tetrahedral, bent, trigonal bi-pyramidal, see saw, T-shape, or octahedral*)
 - c. Bond angle between the atoms attached to the central atom. (Based on the molecular geometry)
 - d. Type of hybridization of the central atom in each molecule – if any (sp, sp², sp³, sp³d)
 4. Construct a 3D model for each compound using the online PhET simulation, and then sketch onto your paper.
 - a. https://phet.colorado.edu/sims/html/molecule-shapes/latest/molecule-shapes_en.html
 - b. **Expectation is that you complete the table WITHOUT using part C first, THEN use part C to correct after. Use your 3D image to sketch in the table**
 - c. Click to turn on the following:
 - Lone pairs
 - Bond angles
 - Electronic and Molecular Geometry
 - d. Click in the bottom right corner where it says “PhET” and there are three vertical dots
 - Click options, then “projector mode” – it makes the background white so it is much easier to see things (I think so at least!).
1. Build molecules for the compounds and complete the table:

Molecular Formula	AXE Formula	Lewis Structure	Electronic Geometry	Bond Angle	3D Sketch
CS ₂		# v.e. =			
# Bond Pairs	Steric Number		Molecular Geometry	Hybridization	
# Lone Pairs					

Molecular Formula	AXE Formula	Lewis Structure	Electronic Geometry	Bond Angle	3D Sketch
HCN		# v.e- =			
# Bond Pairs	Steric Number		Molecular Geometry	Hybridization	
# Lone Pairs					

Molecular Formula	AXE Formula	Lewis Structure	Electronic Geometry	Bond Angle	3D Sketch
SO ₃		# v.e- =			
# Bond Pairs	Steric Number		Molecular Geometry	Hybridization	
# Lone Pairs					

Molecular Formula	AXE Formula	Lewis Structure	Electronic Geometry	Bond Angle	3D Sketch
NO ₂ ⁻		# v.e- =			
# Bond Pairs	Steric Number		Molecular Geometry	Hybridization	
# Lone Pairs					

Molecular Formula	AXE Formula	Lewis Structure	Electronic Geometry	Bond Angle	3D Sketch
CCl ₄		# v.e- =			
# Bond Pairs	Steric Number		Molecular Geometry	Hybridization	
# Lone Pairs					

Molecular Formula	AXE Formula	Lewis Structure	Electronic Geometry	Bond Angle	3D Sketch
NCl ₃		# v.e- =			
# Bond Pairs	Steric Number		Molecular Geometry	Hybridization	
# Lone Pairs					

Molecular Formula	AXE Formula	Lewis Structure	Electronic Geometry	Bond Angle	3D Sketch
H ₂ O		# v.e- =			
# Bond Pairs	Steric Number		Molecular Geometry	Hybridization	
# Lone Pairs					

Molecular Formula	AXE Formula	Lewis Structure	Electronic Geometry	Bond Angle	3D Sketch
TeCl ₄		# v.e- =			
# Bond Pairs	Steric Number		Molecular Geometry	Hybridization	
# Lone Pairs					

Molecular Formula	AXE Formula	Lewis Structure	Electronic Geometry	Bond Angle	3D Sketch
XeF ₂		# v.e- =			
# Bond Pairs	Steric Number		Molecular Geometry	Hybridization	
# Lone Pairs					

Molecular Formula	AXE Formula	Lewis Structure	Electronic Geometry	Bond Angle	3D Sketch
SbCl ₅ ²⁻		# v.e- =			
# Bond Pairs	Steric Number		Molecular Geometry	Hybridization	
# Lone Pairs					

Molecular Formula	AXE Formula	Lewis Structure	Electronic Geometry	Bond Angle	3D Sketch
IOF ₅		# v.e- =			
# Bond Pairs	Steric Number		Molecular Geometry	Hybridization	
# Lone Pairs					

Molecular Formula	AXE Formula	Lewis Structure	Electronic Geometry	Bond Angle	3D Sketch
I ₃ ⁻		# v.e- =			
# Bond Pairs	Steric Number		Molecular Geometry	Hybridization	
# Lone Pairs					

Molecular Formula	AXE Formula	Lewis Structure	Electronic Geometry	Bond Angle	3D Sketch
ICl ₄ ⁻		# v.e- =			
# Bond Pairs	Steric Number		Molecular Geometry	Hybridization	
# Lone Pairs					

Molecular Formula	AXE Formula	Lewis Structure	Electronic Geometry	Bond Angle	3D Sketch
AsF ₅		# v.e- =			
# Bond Pairs	Steric Number		Molecular Geometry	Hybridization	
# Lone Pairs					

Discussion Questions [To be completed on paper and included in your google doc you turn in on GC]

1. Describe the difference between electronic geometry and molecular geometry.
2. Describe the difference between bond polarity and molecular polarity.
3. Explain what makes a molecule polar or nonpolar.
4. Provide an example of each: a polar molecule and a nonpolar molecule, other than those in the lab. Draw their Lewis structures and indicate the polarities of each bond in both examples.
5. Explain using drawings and captions comparing the differences between the 4 types of molecular shapes of compounds with a steric number of 5. Write the chemical formulas for examples of each of those 4 types.