Molecular Shapes Exercise

Objectives

1. Learn to assess bond angles and molecular geometry (or shape) of a species by determining the number of charge clouds around a central atom in a Lewis structure.
2. Determine the polarity (polar or nonpolar nature) of a species.

Introduction

Now that you have practice writing Lewis structures for molecules and ions, we are ready to move to the next step of using those structures to predict certain properties of the species. Determining the three-dimensional shape of a molecule is critical to understanding many properties, including bonding characteristics, polarity, solubility, and phase (gas, liquid, or solid) at room temperature. If we start with Lewis Structures and assume that charge clouds (lone pairs or single/double/triple bonds) repel each other to maximize separation angles, we can make reasonable predictions about molecular geometry.

Determining polarity is a little bit tricky, but there are a few guidelines that work well for our purposes in CHEM 51.

- Assume that all molecules are polar, unless one of the following is true:
  - The species is highly symmetrical with no lone pairs on the central atom. Highly symmetrical in this context means that the shape is linear, trigonal planar, or tetrahedral **and** all peripheral atoms attached to the central atom are the same. Examples include CCl_4, BF_3, and CO_2.
  - Or, the species is a hydrocarbon, meaning that it contains only C and H atoms. Examples include: CH_4, $CH_3CH_2CH_3CH_3$, C_6H_6, and C_8H_{18}.

Procedure

Part 1: Common Molecular Shapes

Using the PhET simulation "Molecular Shapes":

This portion of the activity was adapted from
Kiste et al., *J. Chem. Educ.* 2016, 93, 11, 1900–1903
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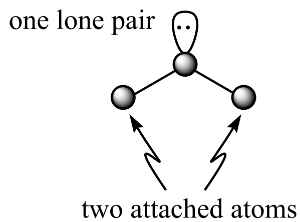
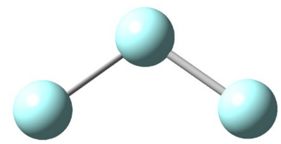
Directions:

Use the "Model" screen on the PhET simulation to explore the shapes of molecules containing various numbers of bonds and lone (nonbonding) pairs of electrons. In this context, the term "charge cloud" refers to any attached atom (single, double, or triple bond) or lone pair. These are simply regions of electron density that repel each other. The number of charge clouds around the central atom is the key factor that determines the shape of the molecule.

As you explore different combinations of bonded atoms and lone pairs, note that the lone pairs influence the positions of the atoms, but the term 'molecular geometry' refers specifically to the resulting shape of the atoms themselves. For example, a central atom with three charge clouds around it might consist of two attached atoms and one lone pair as illustrated below.





In this case, the three charge clouds assume a trigonal planar shape (the "electron pair geometry"), but the atoms themselves assume a bent shape (the "molecular geometry"). In this activity, we will be focusing on molecular geometries.

Use the simulation to complete the tables below to identify the bond angles and molecular geometries of various combinations of attached atoms and lone pairs around a central atom.

Two Charge Clouds

Charge Cloud Combinations	Molecular Geometry	Bond Angles	Sketch
2 attached atoms 0 lone pairs			

Three Charge Clouds

Charge Cloud Combinations	Molecular Geometry	Bond Angles	Sketch
3 attached atoms 0 lone pairs			
2 attached atoms 1 lone pair			

Four Charge Clouds

Charge Cloud Combinations	Molecular Geometry	Bond Angles	Sketch
4 attached atoms 0 lone pairs			
3 attached atoms 1 lone pair			
2 attached atoms 2 lone pairs			

Do your results above change when the atoms are attached with double or triple bonds instead of single bonds?

Part 2: Determining Molecular Shapes and Polarity from Lewis Structures

Using the PhET simulation "Molecular Shapes":

Draw valid Lewis structures for the following six molecules and complete the table below. You may wish to utilize the atom tiles from the 'Covalent Bonding and Lewis Structure' experiment to help. You should continue to use the PhET simulation to model each one, but as you work through these, try to make a prediction for the molecular shape ahead of time. Note that we are only concerned with charge clouds around the central atom – lone pairs on the peripheral atoms are required for a complete Lewis structure, but they are not counted when determining the shape of the central atom.

The geometries should be limited to the list developed above (specifically: linear, bent, trigonal planar, trigonal pyramidal, and tetrahedral). If the simulation shows a geometry not in this list, something is not correct with the model.

Refer to the information provided in the introduction as well as your lecture notes and text book for help in determining the polarity.

Formula	**Lewis Structure**	**# of Charge Clouds**	**# of Attached Atoms**	**# of Lone Pairs**	**Approx. Bond Angle**	**Molecular Geometry**	**Polar or Nonpolar**
1. CO_2							

2. H_2CO							
3. SO_2							
4. CH_4							
5. NF_3							
6. SCl_2							

Part 3: Additional Practice

The following examples provide additional practice drawing Lewis structures and determining geometric properties. As you go through these, you should strive to complete each row using only the Lewis structure you have drawn, though you may still utilize the PhET simulation check your work.

Formula	Lewis Structure	# of Charge Clouds	# of Attached Atoms	# of Lone Pairs	Approx. Bond Angle	Molecular Geometry	Polar or Nonpolar
7. $CHCl_3$							
8. SO_4^{2-}							

9. $SOCl_2$							
10. ClO_2^-							
11. H_2O							
12. SCN^-							
13. SO_3							
14. HCN							
15. $POCl_3$							
16. NO_3^-							
17. O_3							

18. $COCl_2$							
19. AsF_3							
20. NO_2^-							
21. C_3H_8 (answer for each C atom)							
22. C_2H_8O (answer for the O atom)							
23. NO_2^+							
24. C_3H_6 (answer for the central C atom)							
25. C_2H_7N (answer for the N atom)							