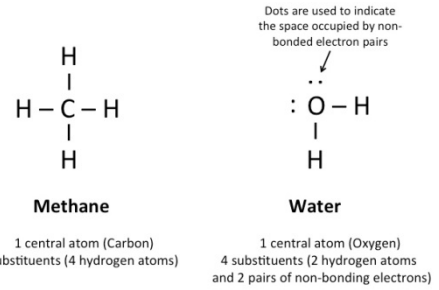
# Lab 2. Molecular Shapes: How Does the Number of Substituents Around a Central Atom Affect the Shape of a Molecule?

## Introduction

Molecules are three-dimensional entities and therefore should be depicted in three dimensions. We can translate the two-dimensional electron dot structure representing a molecule into a more useful three-dimensional rendering by using a tool known as the valance shell electron pair repulsion (VSEPR) model. According to this model, any given pair of valance shell electrons strives to get as far away as possible from all other electron pairs in the shell. This includes both nonbonding pairs of electrons and any bonding pair not taking part in a double or triple bond. Pairs of electrons in a multiple bond stay together because of their mutual attractions for the same two nuclei. It is this striving for maximum separation distance between electron pairs that determines the geometry of any molecule.

### FIGURE L2.1

**Substituents around a central atom**




The VSEPR model allows us to use the electron dot structures of atoms to predict the three-dimensional geometry of simple molecules. This geometry is determined by considering the number of *substituents* surrounding a central atom. A substituent is any bonded atom or nonbonding pair of electrons. For example, the carbon on the methane molecule ($CH_4$) shown in Figure L2.1 has four substituents (four hydrogen atoms). The oxygen atom of water also has four substituents (two hydrogen atoms and two nonbonding pairs of electrons).

## Your Task

Use a computer simulation to develop a rule that you can use to predict the shape of a molecule based on the number of atoms and lone electron pairs (i.e., substituents) around a central atom.

The guiding question of this investigation is, **How does the number of substituents around a central atom affect the shape of a molecule?**

## Materials

You will use an online simulation called *Molecule Shapes* to conduct your investigation. You can access the simulation by going to the following website: *http://phet.colorado.edu/en/simulation/molecule-shapes*.

## Safety Precautions

Follow all normal lab safety rules.

## Investigation Proposal Required? ☐ Yes ☐ No

## Getting Started

The *Molecule Shapes* simulation (see Figure L2.2) models how the number of atoms and lone electron pairs around a central atom affects the shape of a molecule. With this simulation, you can decide how many atoms are found in the molecule, the nature of the bonds found between the atoms (single, double, or triple) and the number of lone electron pairs that are found around the central atom. Your goal is to develop a rule that you can use to predict the shape of a molecule based on the number of atoms and lone

electron pairs (i.e., substituents) found around the central atom. Before you start using the simulation, however, you must determine what type of data you will need to collect, how you will collect the data, and how you will analyze the data to answer the guiding question.

To determine *what type of data you need to collect*, think about the following questions:

- What type of observations will you need to record during your investigation?
- When will you need to make these observations?

To determine *how you will collect the data*, think about the following questions:

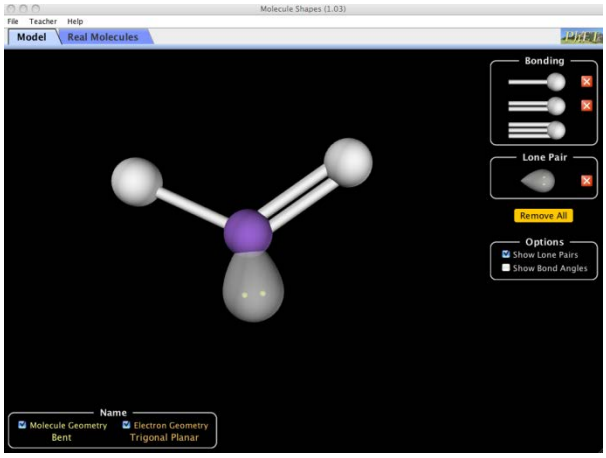
- What types of molecules will you need to examine using the simulation?
- What type of comparisons will you need to make?
- How will you keep track of the data you collect and how will you organize it?

To determine *how you will analyze the data*, think about the following questions:

- What type of calculations will you need to make?
- What type of graph could you create to help make sense of your data?

**FIGURE L2.2**

**A screenshot of the *Molecule Shapes* simulation**




## Connections to Crosscutting Concepts, the Nature of Science, and the Nature of Scientific Inquiry

As you work through your investigation, be sure to think about

- the importance of looking for and identifying patterns,
- how models are used to study natural phenomena,
- how the structure of an object is related to its function,
- the difference between laws and theories in science, and
- the wide range of methods that can be used by scientists during an investigation.

## Initial Argument

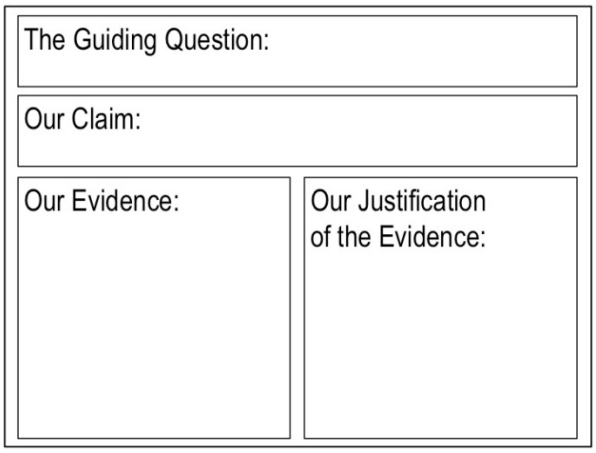
Once your group has finished collecting and analyzing your data, you will need to develop an initial argument. Your argument must include a *claim*, which is your answer to the guiding question. Your argument must also include *evidence* in support of your claim. The evidence is your analysis of the data and your interpretation of what the analysis means. Finally, you must include a *justification* of the evidence in your argument. You will therefore need to use a scientific concept or principle to explain why the evidence that you decided to use is relevant and important. You will create your initial argument on a whiteboard. Your whiteboard must include all the information shown in Figure L2.3.

## Argumentation Session

The argumentation session allows all of the groups to share their arguments. One member of each group stays at the lab station to share that group's argument, while the other members of the group go to the other lab stations one at a time to listen to and critique the arguments developed by their classmates. The goal of the argumentation session is not to convince others that your argument is the best one; rather, the goal is to identify errors or instances of faulty reasoning in the initial arguments so these mistakes can be fixed. You will therefore need to evaluate the content of the claim, the quality of the evidence used to support the claim, and the strength of the justification of the evidence included in each argument that you see. To critique an argument, you might need more information than what is included on the whiteboard. You might therefore need to ask the presenter one or more follow-up questions, such as:

FIGURE L2.3

**Argument presentation on a whiteboard**




- What did your group do to analyze the data, and why did you decide to do it that way?
- Is that the only way to interpret the results of your group's analysis? How do you know that your interpretation of the analysis is appropriate?
- Why did your group decide to present your evidence in that manner?
- What other claims did your group discuss before deciding on that one? Why did you abandon those alternative ideas?
- How confident are you that your group's claim is valid? What could you do to increase your confidence?

Once the argumentation session is complete, you will have a chance to meet with your group and revise your original argument. Your group might need to gather more data or design a way to test one or more alternative claims as part of this process. Remember, your goal at this stage of the investigation is to develop the most valid or acceptable answer to the research question!

## Report

Once you have completed your research, you will need to prepare an *investigation report* that consists of three sections that provide answers to the following questions:

1. What question were you trying to answer and why?
2. What did you do during your investigation and why did you conduct your investigation in this way?
3. What is your argument?

Your report should answer these questions in two pages or less. The report must be typed and any diagrams, figures, or tables should be embedded into the document. Be sure to write in a persuasive style; you are trying to convince others that your claim is acceptable or valid!