ChemActivity 1: Bond Angles and Shape

(What are the bond angles and shape of CH_4?)

Model 1: Planetary Model of an Atom

In a planetary model of an atom, **negatively charged electrons** (–1 each) are arranged around a **positively charged nucleus** (+Z = nuclear charge) in a series of **shells** that look like orbits.

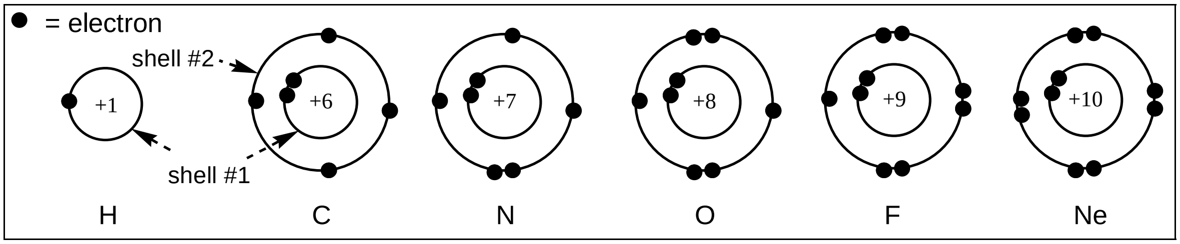


Figure 1.1: Valence Shell Representations of Hydrogen, Carbon, Nitrogen, Oxygen, Fluorine, and Neon

core electrons = electrons in any inner shell(s) (don't participate in bonding)

core atom = the nucleus (made up of protons and neutrons) plus the core electrons

valence electrons = electrons in the outermost shell (participate in bonding)

valence shell = outermost shell, where valence electrons are found

*Electrons **DO NOT** "orbit" the nucleus like the planets orbit the sun. In ChemActivity 3 we will study a more complex model in which electrons are described as inhabiting 3-dimensional regions of space called "orbitals" (1s, 2s, $2p_x$, $2p_y$, $2p_z$, 3s, etc.).*

Critical Thinking Questions

1. (E) What does the number (+Z) at the center of each atom in Figure 1.1 represent, and what number would you expect at the center of a representation of a bromine atom (Br)?

2. (E) How many total electrons does an oxygen atom have, and how could you find the answer to this using a periodic table?

3. (E) How many valence electrons does each atom in Figure 1.1 have, and what number on a periodic table gives you these answers?

4. What is the maximum number of electrons that can fit in…
   a. (E) shell No. 1?
   b. (E) shell No. 2 (Neon has a full Shell No. 2)?
   c. Describe how the answers to a) and b) are contained in the structure of the periodic table.

Model 2: Bonding and Non-bonding Electron Domains

Bonding electron domain = shared valence electrons (2, 4, or 6e⁻) localized between two core atoms

3 types → **Single Bond** (1 pair, 2 electrons); **Double Bond** (2 pairs, 4 e⁻); **Triple Bond** (3 pairs, 6 e⁻)

Non-bonding electron domain (“**lone pair**”) = pair of valence electrons (2 e⁻) not involved in a bond

One way to think of a **bond**: **two positively charged core atoms mutually attracted to the negatively charged electrons that are localized between them**.

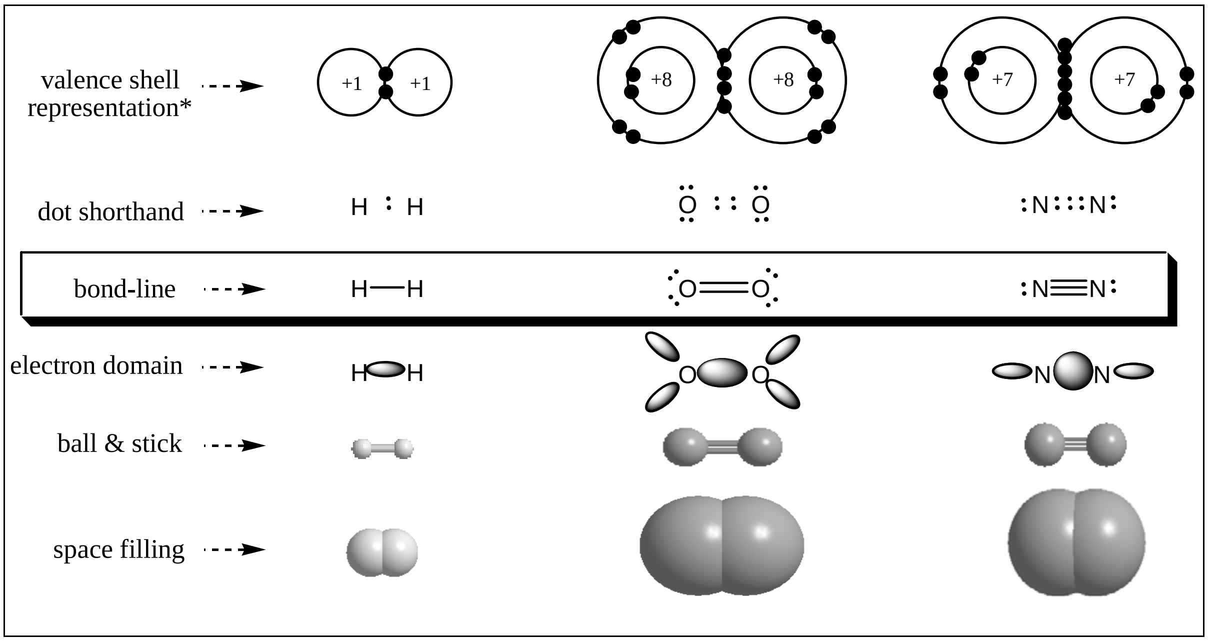


Figure 1.2: Example of a Single, Double, and Triple Bond

Critical Thinking Questions

5. (E) How many electrons are in a triple bond?

6. (E) Identify each **lone pair** shown in the first four rows of Figure 1.2.

7. (E) Each molecule in Figure 1.2 has exactly one bonding electron domain. Identify it and…
   a. label what **type** of bonding electron domain it is.
   b. report the number of electrons in each bonding electron domain.

8. You hear a student from a nearby group say that “E*lectron domains repel one another*.” Cite evidence from Figure 1.2 to support or refute this statement.

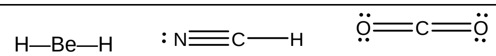
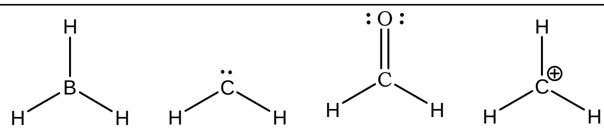
Model 3: Bond Angles

bond angle = angle defined by any three atoms in a molecule. (e.g., ∠HBH in BH_3, below)

According to the Valence Shell Electron Pair Repulsion model (**VSEPR**) **electron domains spread out as far as possible** from one another (repel one another).

Even for a molecule with different-sized electron domains (e.g., H_2CO), bond angles remain very close to those you would expect if all the electron domains were the same size.

Table 1.1: Bond Angles of Selected Molecules

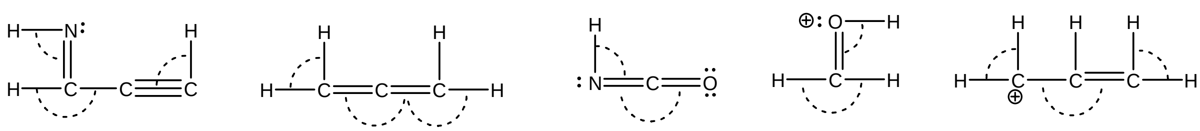
Bond-line Structure	Approximate Bond Angle
	180
	120

Critical Thinking Questions

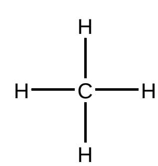
9. Use VSEPR to explain why the ∠HBH bond angle of BH_3 is 120°. (*Hint*: What is one-third of 360°?)

10. Both the ∠HCH and ∠HCO bond angles of H_2CO (formaldehyde) are very close to 120°, but one is slightly smaller than the other. Predict which is smaller, and explain your reasoning.

11. Use VSEPR to assign a value of "**close to 180°**" or "**close to 120°**" to each bond angle marked with a dotted line. (These angles are drawn as either 90° or 180°, but may be another value.)

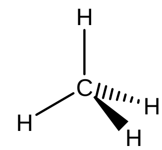


12. Consider the following **flat** drawing of methane (CH_4).



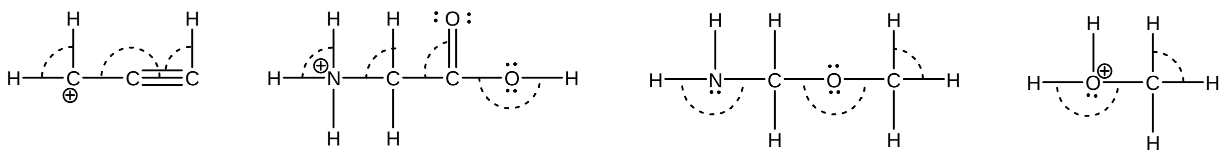
   a. What is ∠HCH bond angle implied by this drawing if you assume it is flat?
   b. Are the electron domains of this flat CH_4 spread out as much as possible?
   c. Use model materials to **make a model of CH_4** (methane). If you assembled it correctly, the four bonds (bonding electron domains) of your model will be 109.5° apart.
   d. In which representation, **the drawing above** or **the model in your hand** (circle one) are the H's of CH_4 more spread out around the central carbon?

e. Confirm that your model looks like the following drawing. The **wedge bond** represents a bond coming out of the page, and the **dash bond** represents a bond going into the page.

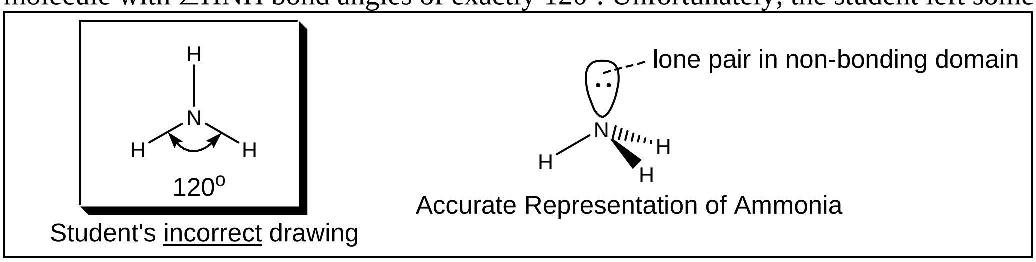


f. You will often see methane drawn as if it were flat (like on the previous page). Why is this misleading, and what is left to the viewer's imagination when looking at such a drawing?

13. Use VSEPR to assign a value of (close to) 109.5, 180 or 120 to each marked **bond angle**.



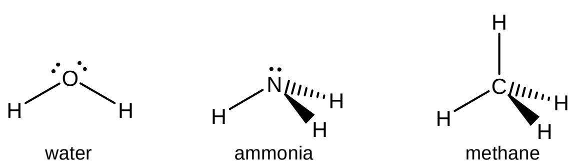
14. A student draws the picture of **ammonia** (NH_3) in the box below, left, and predicts it will be a flat molecule with ∠HNH bond angles of exactly 120°. Unfortunately, the student left something out.



a. What did the student omit from his drawing?

b. What is the actual ∠HNH bond angle of ammonia (based on the drawing above, right)?

c. Explain why water, ammonia, and methane (shown below) all have about the same bond angles (close to 109.5°) even though they have different numbers of bonds.



Memorization Task 1.1: Correlation between #No. of Electron Domains and Bond Angle

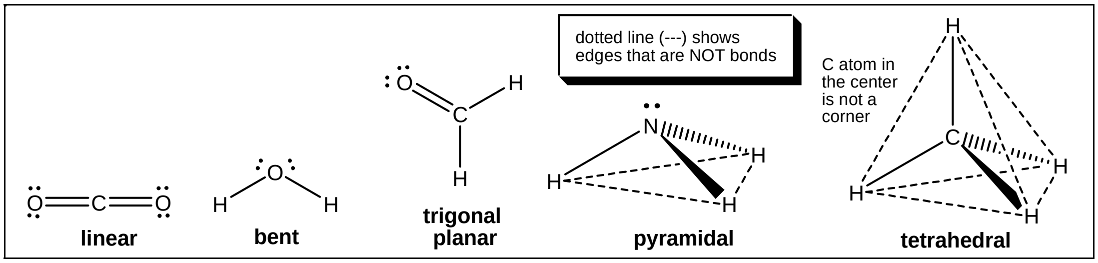
Electron Domains (bonding + non-bonding)	Bond Angle Close To…	Examples
4	109.5°	CH_4, NH_3, H_2O, H_4N^+
3	120°	BH_3, H_3C^+, CH_2, H_2CO
2	180°	BeH_2, O_2N^+, CO_2, HCN

Model 4: Shape

A **central atom** = an **atom bonded to two or more other atoms**. (e.g., Oxygen in H—O—H)

Each **central atom** has a **shape** determined by the arrangement of the **atoms** attached to it.

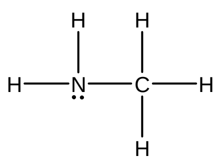
Memorization Task 1.2: The five molecular shapes we will encounter in this course



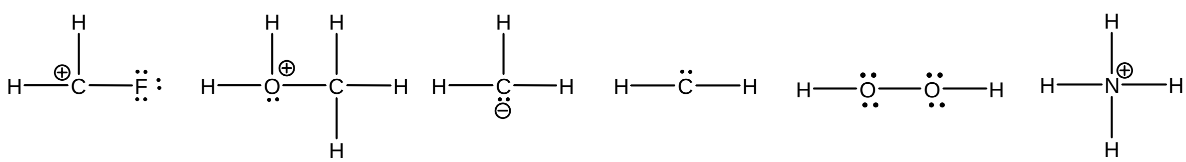
Critical Thinking Questions

15. (E) Explain why the molecule H—F is not associated with an official shape as defined in Model 4.

16. How many central atoms does the molecule H_2NCH_3 have, and what is the shape about each?



17. Indicate the bond angle and shape about each central atom.



18. Explain how there can be two kinds of bent: "**bent-109.5o**" and "**bent-120o**," and give an example of each from the previous question. (Note that "bent-109.5^{o}" is more common than "bent-120^{o}.")

19. A student makes the following statement: "The shape of water is **tetrahedral** because the four electron pairs about oxygen are approximately 109.5^{o} apart and point to the corners of a tetrahedron." What misconception does this statement convey?

20. A student who missed this class needs to know how to predict the bond angles and shape of a molecule from looking at its bond-line representation. Write a concise but complete explanation for this student.

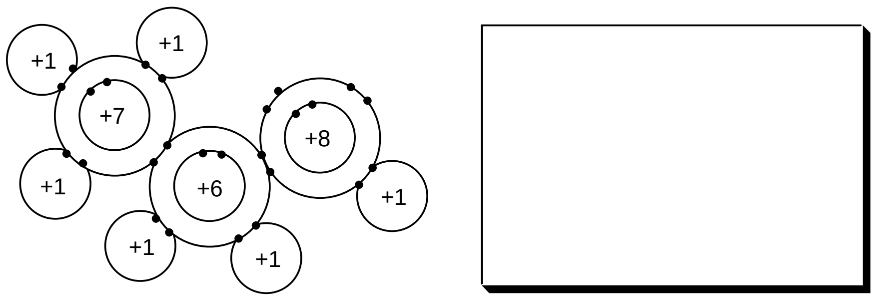
Exercises

1. Draw a valence shell representation of a

   a. Helium atom.

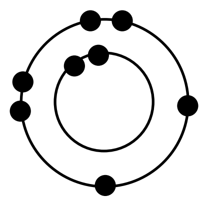
   b. Sulfur atom.

2. In the box, draw a **bond-line representation** of the molecule shown on the left. Be sure to include <u>only</u> valence electrons (either as line bonds or lone pairs).



line-bond rep.

3. Consider the incomplete valence shell representation below.



   a. Assume the atom is neutral, and write the correct nuclear charge at the center of the atom.

   b. What is the identity of this neutral atom?

4. How many valence electrons does a neutral

   a. K atom have?

   b. C atom? N atom? O atom?

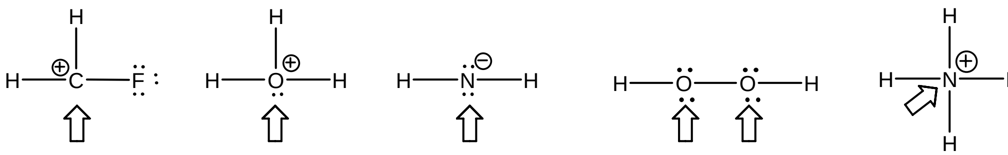
5. Consider the molecules $AlCl_3$ (aluminum chloride) and CF_4 (carbon tetrafluoride).

   a. Draw the valence shell representation of each.

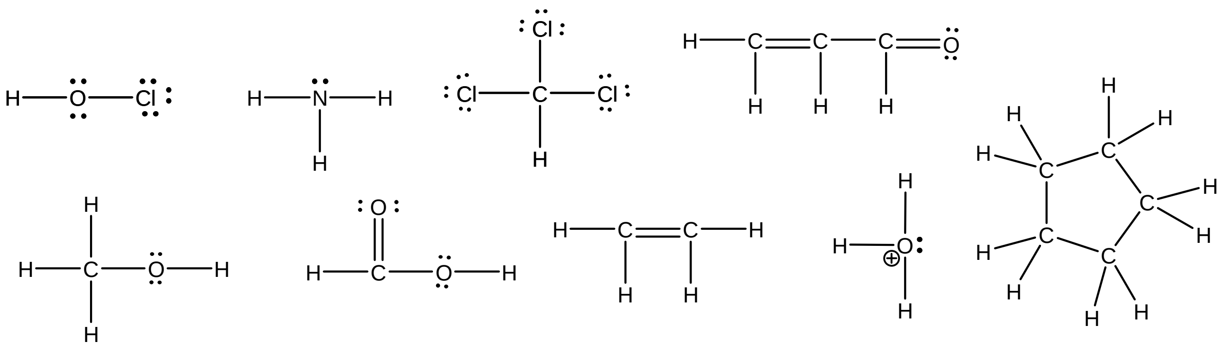
   b. Predict the value of the XYX bond angle, and explain your reasoning.

6. Draw an example of a bent molecule with a bond angle of near 109.5^{o}; then draw a different bent molecule with a bond angle of about 120^{o}.

7. Label each atom marked with an arrow with the appropriate **shape name,** and **estimate the bond angles around it** as being close to one of 180^o, 120^o, 109.5^o or 90^o. (circled charges indicate the charge on the molecule or fragment)



8. Make a model of each of the following molecules:



a. Based on your model, draw a bond-line representation with as many atoms as possible in the plane of the paper. Use wedge and dash bonds to represent any atoms that do not lie in the plane of the paper.

b. Indicate each unique bond angle and the shape of each unique central atom.

9. Read the assigned pages in the text, and do the assigned problems.

Using "The Big Picture" & "Common Points of Confusion" Sections

It can be fun to "discover" your own answers as you are asked to do in this workbook, but…

How do you know if your "discovered" understanding is valid?

The answer is: Even practicing scientists and professors never know *for sure* that they are correct. In some ways, deciding if you are right is the hardest part of being a scientist. A practicing scientist cannot "check the key" to see if her new theory is correct! In this course and in real life you must constantly test and improve your current understanding by applying it to problems and discussing it with peers. One goal of this course is to develop the ability to recognize the signs when you are correct; and equally importantly, recognize the signs when you are missing something critical.

After completing a ChemActivity, one way to start checking your understanding is to read the Big Picture and Common Points of Confusion sections (examples on the next page). If the homework or these sections do not make sense to you then you are missing something important. You need to go back and study the activity, do more problems, read the textbook more closely, or seek help from a peer, teaching assistant or your instructor. (More advice about how to know if you are "**learning the right thing**" can be found in the "To the Student" section the precedes the Table of Contents for this book, and the Frequently Asked Questions section of the IntroActivity that precedes this chapter.)

The Big Picture

After this week you will rarely be asked to report a bond angle or shape. Yet it is critical that you be able to do both. Doing well in organic chemistry largely depends on your ability to see molecules as three-dimensional objects. The electrons of most every central atom you will encounter are arranged 109.5^{o} or 120^{o} apart (180^{o} arrangements are quite rare), but it gets complex when you are expected to see a molecule with multiple central atoms in 3D. The purpose of this activity is to get you started thinking about tetrahedral and trigonal planar geometries. If you do not already have a model set, borrow or purchase one. You will need it for the first half of this course while you are "programming" your brain to see the two-dimensional drawings on the page as 3D objects.

Common Points of Confusion

At the end of each chapter you will find a brief explanation of common student misconceptions. This section may be useful if a homework problem does not make sense or as final preparation for a quiz.

- When asked the question, "What is the **shape** of water?" students sometimes answer "tetrahedral" because they know that the four electron domains of water spread out into a tetrahedral-type pattern. However, the answer is "bent" because shape is determined by the location of the atoms. Similarly, it makes no sense to ask what is the bond angle between the two lone pairs of water—there should be approximately 109.5^{o} between these lone pairs, but this is difficult to measure.
- Some students mistakenly assume they are expected to predict the EXACT **bond angle** of a given molecule. Generally, you are expected to predict only if the bond angle is closest to 180, 120, or 109.5 degrees.