What Shapes Do Molecules Have?

Why are we doing this?

The Lewis structure provides a good model to describe the connectivity of molecules. However, the two-dimensional Lewis structures do not do a good job of explain or showing the three-dimensional shape of the molecule. Using the concepts of electron domains and electron-electron repulsion, we can predict the molecular shapes that we observe for molecules.

Your Learning Outcomes

You will be able to:
1. Determine the number of electron domains in a molecule from its Lewis structure.
2. Predict the ideal bond angle between atoms in a molecule using the concept of electron-electron repulsion between electron domains.
3. Identify the molecular shape (also called molecular geometry) of a molecule.

The Plan

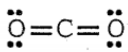
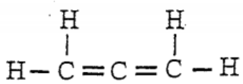
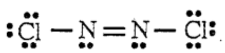
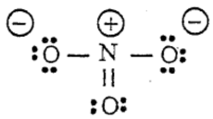
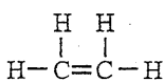
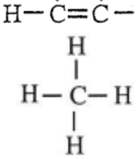
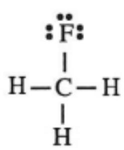
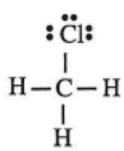
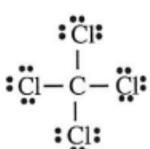
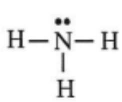
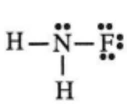
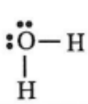
1. Assign roles*.
    a. ***Manager*** – This person will keep the team on task and provide direction to the group. This person is responsible for uploading the group's work to Gradescope. Make sure you make a note of everyone in the group. You must add everyone's name when submitting your answers to Gradescope.
    b. ***Spokesperson*** – This person will represent the group be responsible for speaking for the group to the rest of the class.
    c. ***Recorder*** – This person will be responsible for recording the team's answers to the Critical Thinking Questions in an organized and coherent manner.
    d. ***Analyst*** – This person will be responsible for critical analysis of the team's work (i.e., the Devil's Advocate). This person should make sure everyone understands what is happening before the group moves forward.
2. Complete the Critical Thinking Questions as a group.
3. Submit your team's work via Gradescope. Groups may choose to work in a Word document or write out their answers on a separate sheet of paper. All work must be upload to Gradescope as a PDF file.

**Students may choose to complete this activity independently if they are unable to attend discussion due to illness or injury; in which case, the student must perform all roles and complete all aspect of the activity. To receive full credit, documentation as to the need for the absence from discussion must be included with the submission and your TA must be notified of the absence.*

Model 1: Bond Angle and Electron Domains.

A **bond angle** is the angle made by three connected nuclei in a molecule. By convention, the bond angle is considered to be between 0° and 180°.

Table 1. Bond angles and bonding domains in selected molecules.

Molecular Formula	Lewis Structure	Bond Angle (calculated)	No. of Bonding Domains (central atom)	No. of Nonbonding Domains (central atom)
CO_2		∠OCO = 180°	2	0
HCCH		∠HCC = 180°	2	0
H_2CCCH_2		∠CCC = 180°	2	0
ClNNCl		∠ClNN = 117.4°	2	1
NO_3^-		∠ONO = 120°	3	0
H_2CCH_2		∠HCH = 121.1°	3	0
CH_4		∠HCH = 109.45°	4	0
CH_3F		∠HCH = 109.45° ∠HCF = 109.45°	4	0
CH_3Cl		∠HCH = 109.45° ∠HCCl = 109.45°	4	0
CCl_4		∠ClCCl = 109.45°	4	0
NH_3		∠HNH = 107°	3	1
NH_2F		∠HNH =106.95° ∠HNF = 106.46°	3	1
H_2O		∠HOH = 104.5°	2	2

Critical Thinking Questions

1. For each molecule below, complete the table based on the information in Table 1.

Molecule	Central Atom	Number of atoms bonded to a central atom	Number of lone pairs of electrons on a central atom
CO_2	C	2	0
ClNNCl	N	2	1
NH_3	N	3	1

2.
   a. How is the number of bonding domains on a given atom within a molecule (such as those in Table 1) determined?
   The number of bonding domains is equal to the number of bonded atoms (to the given atom).

   b. How is the number of nonbonding domains on a given atom with a molecule (such as those in Table 1) determined?
   The number of nonbonding domains is equal to the number of lone pairs on the given atom.

3. The bond angles in Table 1 can be grouped, roughly, around three values. What are these three values?
180, 120, 109

4. What correlation can be made between the values in the last two columns in Table 1 and the groupings identified in Question 3?
When the sum of the number of bonding and nonbonding domains is 2, the angle is 180°.
When it is 3, the angle is about 120°.
When it is 4, the angle is about 109°.

Model 2: Models for Methane, Ammonia, and Water.

Use a molecular modeling set to make the following molecules: CH_4, NH_3, H_2O. (In many modeling kits: carbon is black; oxygen is red; nitrogen is blue; hydrogen is white. Nonbonding electrons are not represented in these models.) If you don't have access to a modeling kit, please use the following PhET simulation (select the Real Molecules application, and then investigate the structures of CH_4, NH_3, and H_2O).

https://phet.colorado.edu/sims/html/molecule-shapes/latest/molecule-shapes_en.html

Critical Thinking Questions

5. Sketch a picture of the following molecules based on your models:
   a. CH_4

   b. NH_3

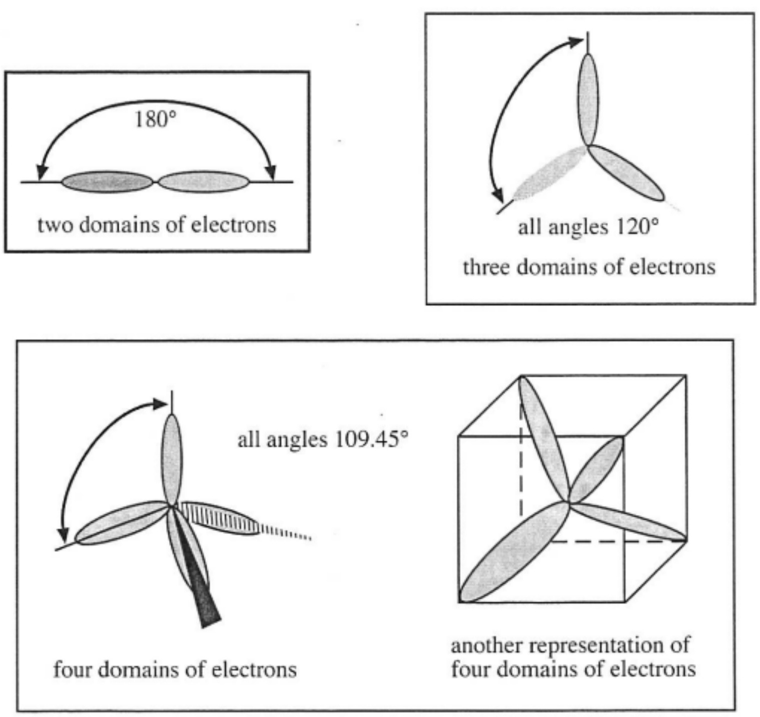
   c. H_2O

6. Describe (with a word or short phrase) the shape of each of these molecules:
   a. CH_4
      Answers will vary but should describe the general shape observed.
   b. NH_3
      Answers will vary but should describe the general shape observed.
   c. H_2O
      Answers will vary but should describe the general shape observed.

Model 3: Types of Electron Domains

A domain of electrons (two electrons in a nonbonding domain—sometimes called a lone pair, two electrons in a single bond domain, four electrons in a double bond domain, or six electrons in a triple bond domain) tend to repel other domains of electrons. Domains of electrons around a central atom will orient themselves to minimize the electron-electron repulsion between domains.

Figure 1. Minimization of electron-electron repulsion leads to a unique geometry for two, three and four domains of electrons.



Critical Thinking Questions

7. Based on Figure 1, what bond angle is expected for a molecule containing:
   a. Two domains of electrons?
   180°
   b. Three domains of electrons?
   120°
   c. Four domains of electrons?
   109°
8. Complete the table below.

Molecular Formula	Lewis Structure	Total number of electron domains	Predicted bond angle (from Figure 1)	Calculated bond angle (from Table 1)
CH_4		4	109.45°	109.45°
NH_3		4	109.45°	107°
H_2O		4	109.45°	104.5°
NO_3^-		3	120°	120°
CO_2		2	180°	180°

9. Individually, determine which of the following statements appears to be true. There may be more than one. Then, reach consensus with your group members.
   a. When a central atom has no lone pairs, the bond angle predicted by the Lewis structure is equal to the observed (calculated) bond angle.
   True
   b. When the central atom has one or more lone pairs, the bond angle predicted by the Lewis structure is slightly larger than the observed (calculated) bond angle.
   False
   c. When the central atom has one or more lone pairs, the bond angle predicted by the Lewis structure is slightly smaller than the observed (calculated) bond angle.
   True

10. Based on your answer to Question 9, predict the bond angle for each of these species:
    a. O_3
    Slightly less than 120°

    b. H_2CO
    About 120°

    c. NH_2F
    Slightly less than 109.45°

Information

The names for the molecular shapes are based on the position of the atoms in the molecule—not on the position of the electron domains.

Figure 2. The Lewis structure, electron domains, and molecular shape of H_2O.

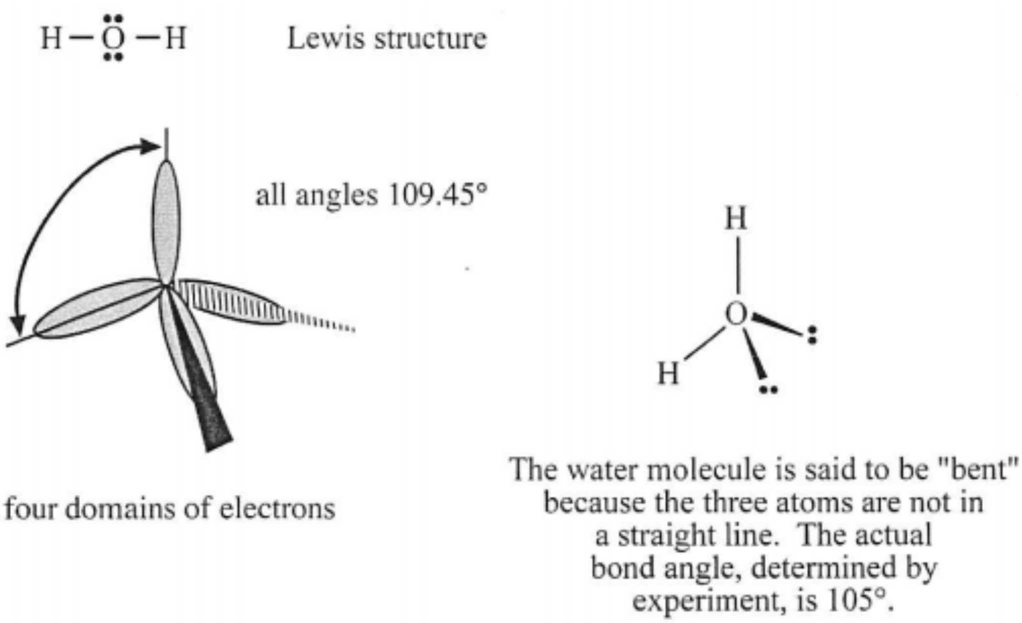
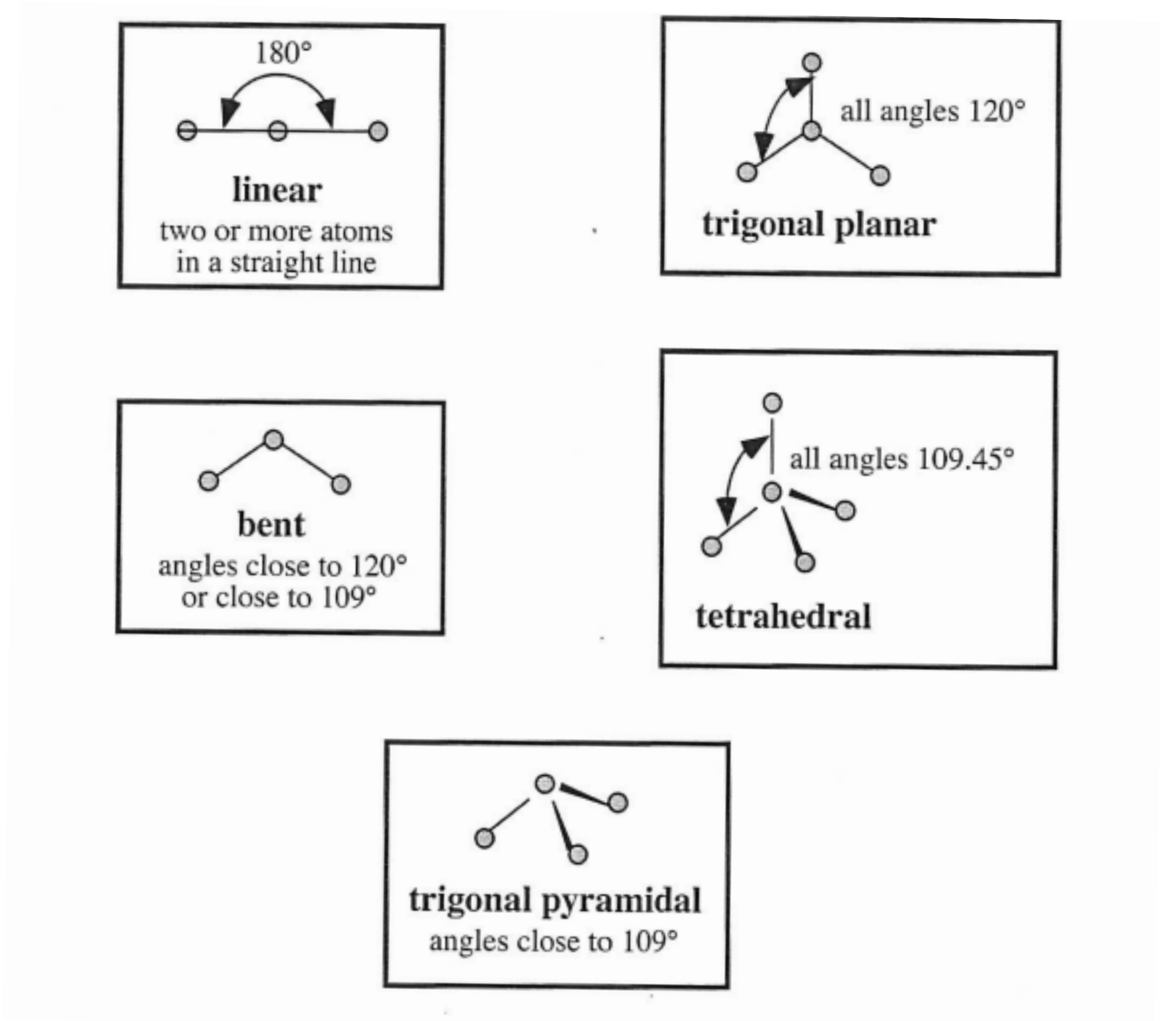


Figure 3. Five common molecular shapes.



Critical Thinking Questions

11. Considering the geometries described in Figure 1, explain why the bond angle in bent molecules is expected to be close to either 109° or 120°.
    If there are more than two bonding domains, minimization of electron-electron repulsion results in bond angles close to 120° (three domains) or 109° (four domains).

12. Explain how the shape of a molecule can be predicted from its Lewis structure.
    i) Determine the total number of electron domains around the atom in question.
    ii) If there are two bonding domains, the molecule will be linear.
    iii) If there are three bonding domains, the molecule will be trigonal planar (when there are three atoms bonded) or bent (when there are two atoms bonded) or linear (when there is only one bonded atom).
    iv) If there are four bonding domains, the molecule will be tetrahedral (when there are four atoms bonded) or trigonal pyramidal (when there are three atoms bonded) or bent (when there are two atoms bonded) or linear (when there is only one bonded atom).