LESSON

10 Two's Company

Electron Domains

Think About It

You may have noticed that there are a certain number of holes in the atoms in the molecular model kits and that the sticks can go only in certain places. So, when you connect the atoms, the molecules automatically end up with the correct three-dimensional shape. But what is it that determines the actual shape of a molecule?

How do electrons affect the shape of a molecule?

To answer this question, you will explore

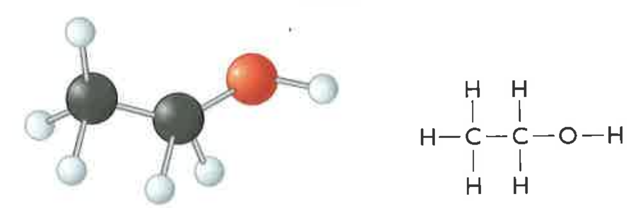
1. Shapes of Molecules
2. Electron Domains

Exploring the Topic

1 Shapes of Molecules

These illustrations show models of ethanol, C_2H_6O.

Ethanol

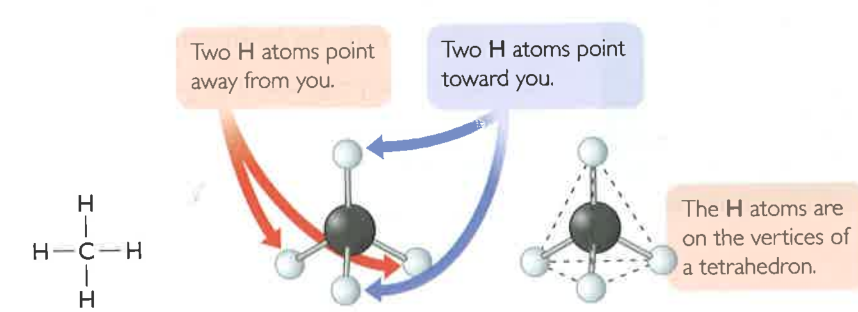


Ball-and-stick model

Structural formula

What accounts for the three-dimensional structure of ethanol? The answer lies in the valence electrons. They determine the ultimate shape of a molecule.

To understand molecular shape, it is useful to begin by examining a simple molecule such as methane, CH_4. While the structural formula is flat and looks like a cross, the ball-and-stick model shows that methane has a three-dimensional structure. Both models show that there are four bonds.



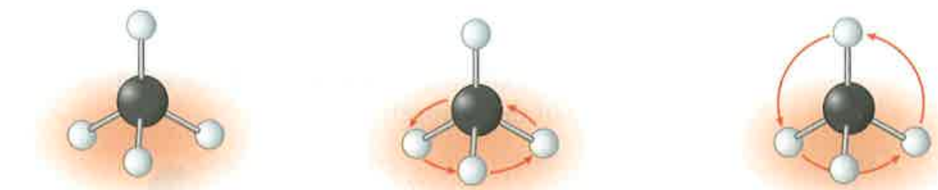
Structural formula

Ball-and-stick model

Tetrahedral

The word used to describe the shape of the methane molecule is **tetrahedral.** A tetrahedral molecule has a symmetrical shape, with one atom exactly in the center. The distance between any other two atoms bonded to the central atom is the same.

You can prove to yourself that a ball-and-stick model of methane is symmetrical in every direction by spinning the molecule as shown in the illustrations. The molecule looks exactly the same no matter what direction it is spun.



One H atom sticks straight up. Three H atoms rest on the table.

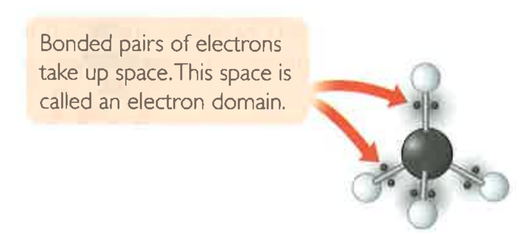
You can spin the molecule around and it looks identical.

You can grab one of the H atoms on the table and spin the molecule around and it still looks identical.

2 Electron Domains

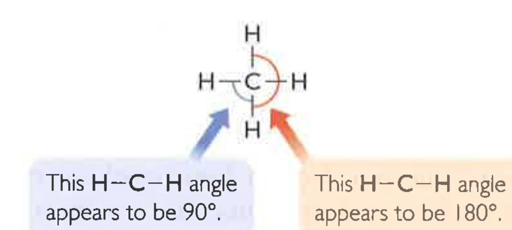
Methane, CH_4

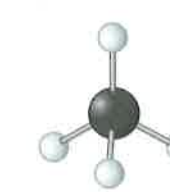
The illustration here shows a methane molecule with the shared valence electrons superimposed, or laid, over the ball-and-stick model. The bonded electron pairs occupy space between the carbon atom and each of the four hydrogen atoms. The space occupied by the electrons is called an **electron domain.** An electron domain can consist of a bonded pair of electrons, a lone pair of electrons, or multiple bonded pairs of electrons.



A methane molecule has four electron domains.

Each electron domain in the tetrahedral methane molecule is the same distance from the other three electron domains. They are as far apart from one another as possible. Because of this, the hydrogen atoms are as far apart from one another as possible. The distance between any two hydrogen atoms is the same. In addition, if you measured the angles formed between any two hydrogen atoms and the carbon atom, all the bond angles would be the same for this tetrahedral molecule. This is not accurately shown in the structural formula.





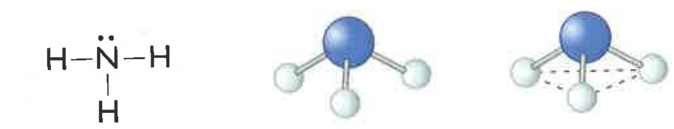
Each H—C—H bond angle is actually 109°.

This tendency for electron pairs to be as far apart from one another as possible is called **electron domain theory.** This theory is also referred to as valence shell electron pair repulsion theory, or *VSEPR.*

Important to Know Electrons are negatively charged, so they repel one another. However, in molecules, electrons bond in pairs. It is the electron pairs that repel one another. ◂

Ammonia, NH_3

The structural formula and ball-and-stick model for ammonia, NH_3, are shown below. The ball-and-stick model shows that the hydrogen atoms are all located on one side of the nitrogen atom.

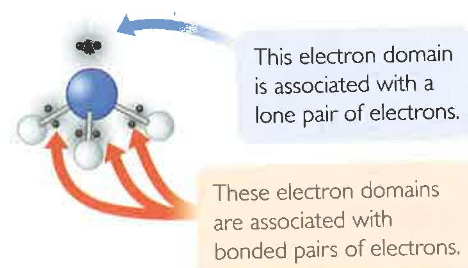


Structural formula Ball-and-stick model Pyramidal

The word used to describe the shape of the ammonia molecule is **pyramidal.**

The nitrogen atom has a lone pair of electrons. Therefore, while there are only three bonds, there are four electron domains. The four electron domains are arranged in a tetrahedral shape to get as far apart as possible, similar to what happens in methane.

An ammonia molecule has four electron domains, just like methane.



Water, H_2O

Take a look at one more molecule—water, H_2O. The word used to describe the shape of a water molecule is **bent.**

Structural formula Ball-and-stick model

A water molecule has four electron domains, two bonding pairs and two lone pairs. The four electron domains of water are arranged in a tetrahedral shape, as in methane and ammonia. This results in a bent shape for the water molecule. In all three molecules, the bond angles are 109° or close to this.

INDUSTRY CONNECTION

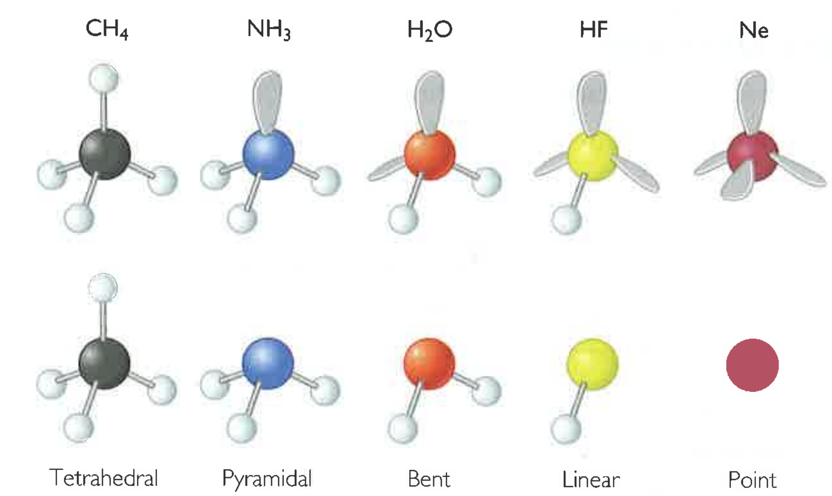
Phosphine is a highly toxic, highly flammable, colorless gas used as a fumigant to kill insects that might damage stored grain.

Bent

A molecule of water has four electron domains, just like methane.

Ball-and-Stick Models with Lone Pair Paddles

In a molecular model kit, the lone pairs are sometimes represented as plastic paddles. This helps you to visualize where the final shape of a molecule comes from.



Notice that you name the shape of the molecule based only on the arrangement of atoms. The lone pairs are not considered.

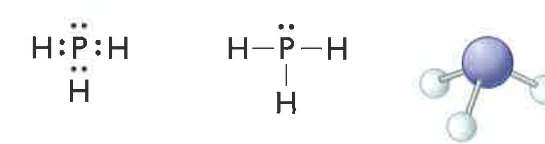
Example

Phosphine, PH_3

What is the shape of phosphine, PH_3? Explain your thinking.

Solution

Begin by drawing the Lewis dot structure and a structural formula with lone pairs of phosphine. A phosphorus atom has five valence electrons and each hydrogen atom contributes one electron, for a total of eight electrons. There are three bonding pairs and one lone pair. The four atoms in phosphine are arranged in a pyramidal shape.



Key Terms

tetrahedral shape
electron domain
electron domain theory
pyramidal shape
bent shape

Lesson Summary

How do electrons affect the shape of a molecule?

The three-dimensional shape of a molecule is determined by the various electron pairs in the molecule. *Both* bonded pairs of electrons *and* lone pairs of electrons affect the shape of a molecule. Each electron pair takes up space, called an electron domain. The final shape of a molecule is determined by the fact that electron domains in a molecule are located as far apart from one another as possible.

EXERCISES

#3, 4, 7

Reading Questions

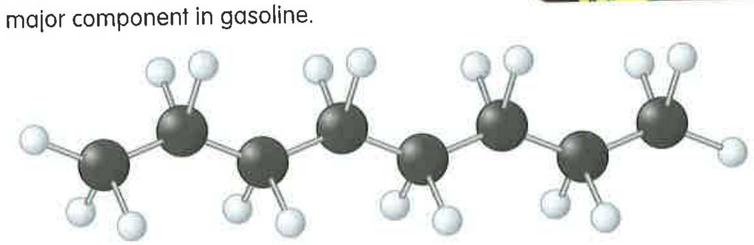
1. In your own words, describe a tetrahedral shape.
2. What is meant by electron domain theory?

Reason and Apply

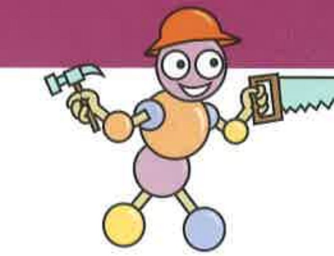
3. If you were going to predict the three-dimensional structure of a small molecule, what would you want to know?
4. Predict the three-dimensional structure of H_2S. Explain your thinking.
5. List three molecules that have a tetrahedral shape.
6. List three molecules that have a bent shape.
7. What is the shape of arsine, AsH_3? Explain your thinking.
8. Predict the three-dimensional shape of HOCl. Explain your thinking.
9. Draw a methane, CH_4, molecule and show how it fits inside a tetrahedron. Do the same for ammonia, NH_3, and water, H_2O.

CONSUMER CONNECTION

Molecules containing *only* carbon and hydrogen atoms are generally referred to as hydrocarbons. The simplest hydrocarbon compound is methane. Notice that methane's name ends in "-ane" because it is an alkane. Many of the medium-sized alkane molecules smell like octane, a major component in gasoline.



Octane



LESSON 11

Let's Build It

Molecular Shape

Think About It

So far you have considered the shapes of small molecules containing single bonds. All of the molecules you've studied have had four electron domains. However, small molecules that have only three or even two electron domains also exist. These molecules have double and triple bonds. So, there are more molecular shapes to consider.

How can you predict the shape of a molecule?

To answer this question, you will explore

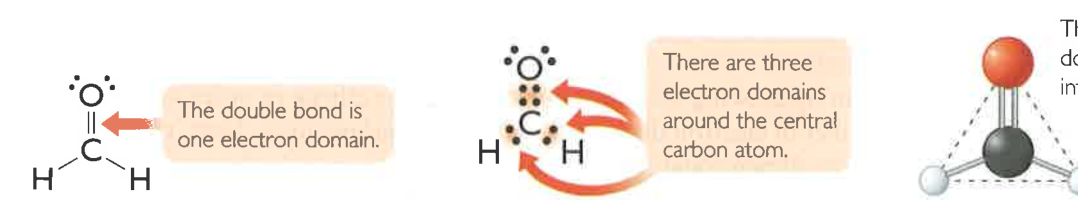
1. More Shapes
2. Larger Molecules

Exploring the Topic

1 More Shapes

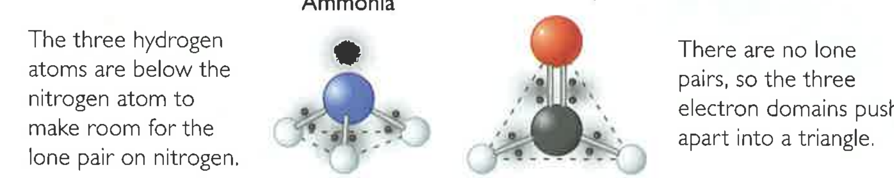
Double Bonds

Formaldehyde, CH_2O, is a very simple molecule that contains one double bond. The double bond counts as only one electron domain even though it contains two pairs of bonded electrons. This means that the central atom in the formaldehyde molecule (the carbon atom) has only three electron domains surrounding it, spread out into a flat triangle. The phrase used to describe the underlying shape of the formaldehyde molecule is **trigonal planar.**



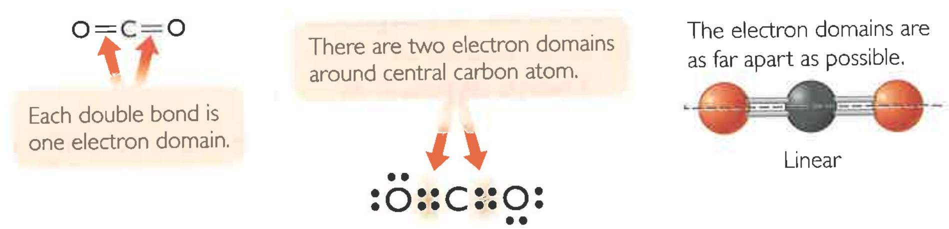
Structural formula Lewis dot structure Trigonal planar

Both ammonia, NH_3, and formaldehyde, CH_2O, have four atoms but have very different shapes. The difference in shape is due to the number of electron domains around the central atom.



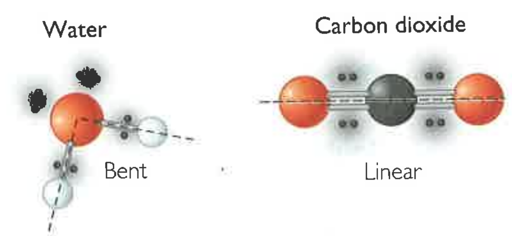
Two Double Bonds

In a molecule with a double bond, the double bond counts as one electron domain. So a molecule like carbon dioxide, with two double bonds, has only two electron domains around the central atom and they need to be as far apart as possible. This shape is described as **linear.**



Important to Know The four electrons in a double bond remain between two atoms, so they are considered one electron domain. An electron domain can have two, four, or six electrons. ◂

Both water, H_2O, and carbon dioxide, CO_2, have three atoms. However, the shape of water is bent while carbon dioxide is linear. The difference in shape is due to the number of electron domains around the central atom.



INDUSTRY CONNECTION

Ethene, C_2H_4, is also called ethylene. It is a colorless gas with a slightly sweet odor. Ethene is used in the manufacture of many common products like polyethylene plastic and polystyrene. Ethene also can be used as a plant hormone to control the ripening of fruit or the opening of flowers.

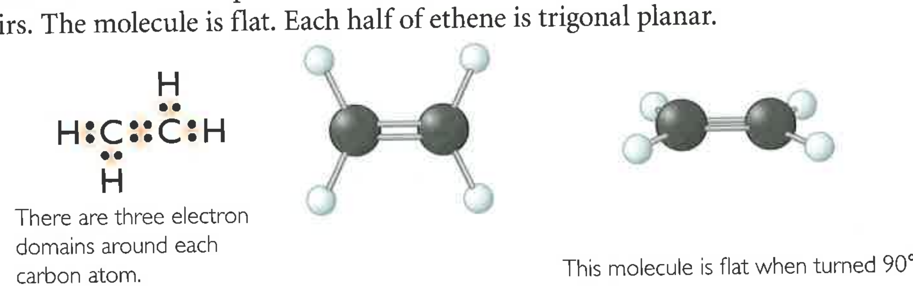
Example 1

Ethene, C_2H_4

Determine the molecular shape of ethene, C_2H_4.

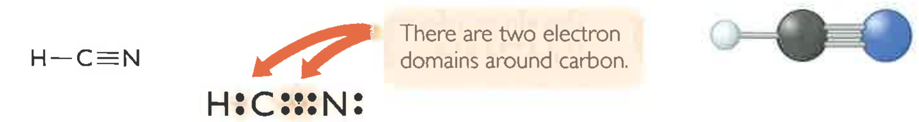
Solution

Begin by drawing the Lewis dot structure for ethene in order to determine the number of electron domains around each carbon atom. Next, translate that into a three-dimensional representation of the molecule. In this case, there are no lone pairs. The molecule is flat. Each half of ethene is trigonal planar.



Triple Bonds

Another example of a linear molecule is hydrogen cyanide, HCN. It also has two electron domains around the central atom, like carbon dioxide. One electron domain is a single bond between carbon and hydrogen, and the other is a triple bond between carbon and nitrogen.



Hydrogen cyanide has one single bond and one triple bond. This results in two electron domains around the central atom.

INDUSTRY CONNECTION

Ethyne, C_2H_2, is also called acetylene. It is the highly flammable gas used by welders in oxyacetylene torches. Miners' helmets used to have carbide lamps attached to them. A carbide lamp is based on the reaction between calcium carbide, CaC_2, and water, H_2O, to produce acetylene, C_2H_2. The acetylene gas burns to produce a bright light in the dark cave.

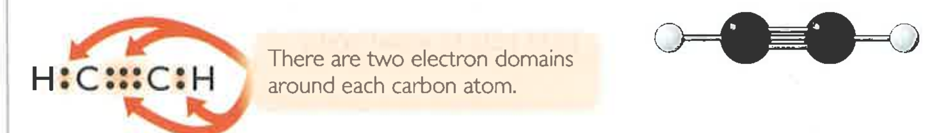
Example 2

Ethyne, C_2H_2

Determine the molecular shape of ethyne, C_2H_2.

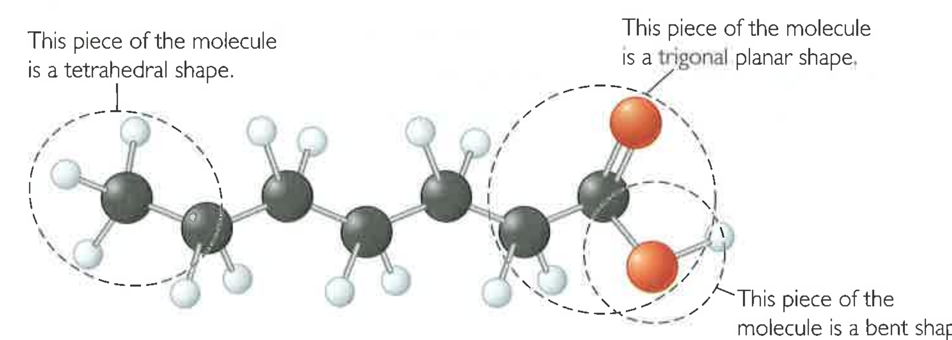
Solution

Begin by drawing the Lewis dot structure of ethyne in order to determine the number of electron domains around the carbon atoms. In order to satisfy the octet rule and the HONC 1234 rule, the carbon atoms must have a triple bond between them. Each carbon atom has two electron domains surrounding it. Ethyne is a linear molecule.



2 Larger Molecules

The shapes of all of these small molecules help to explain why chains of carbon atoms are crooked rather than straight. The illustration shows a ball-and-stick model for heptanoic acid, $C_7H_{14}O_2$, with seven carbon atoms in a chain. The arrangement of atoms around six of the carbon atoms is tetrahedral. Most of the molecule is a series of overlapping tetrahedral shapes.



Heptanoic acid, $C_7H_{14}O_2$

The various electron domains in this molecule cause its overall shape to be crooked, or zigzag.

Key Terms

trigonal planar shape
linear shape

Lesson Summary

How can you predict the shape of a molecule?

The shape of a molecule is affected by the location and number of its electron domains. Lewis dot structures help you to determine the number of electron domains in a molecule. An atom involved in a double bond or triple bond will have fewer electron domains surrounding it. This results in molecules that have trigonal planar and linear shapes. Large molecules can have various geometric shapes within them. Areas around double bonds are flat and those around triple bonds are linear.

EXERCISES

Reading Questions

1. What shapes are possible if a molecule has three electron domains?
2. What shapes are possible for a molecule with three atoms? Explain your thinking.

Reason and Apply

3. Describe the shape of each of these molecules. (Use Lewis dot structures, the periodic table, and the HONC 1234 rule to assist you.)

   Cl_2 CO_2 H_2O
4. Which of the molecules in Exercise 3 have the same shape?
5. What shape or shapes do you predict for a molecule with two atoms? A molecule with three atoms? Four atoms? Five atoms? You can draw Lewis dot structures or electron domains to assist you in answering the questions.
6. Predict the shapes of these molecules:

   CF_4 NF_3 H_2Se H_2CS
7. Consider the butane, C_4H_{10}, molecule.
   a. Draw the Lewis dot structure for butane.
   b. How many electron domains does the molecule have?
   c. What shape would you predict for C_4H_{10}?
   d. Explain why the carbon atom chain is not straight.

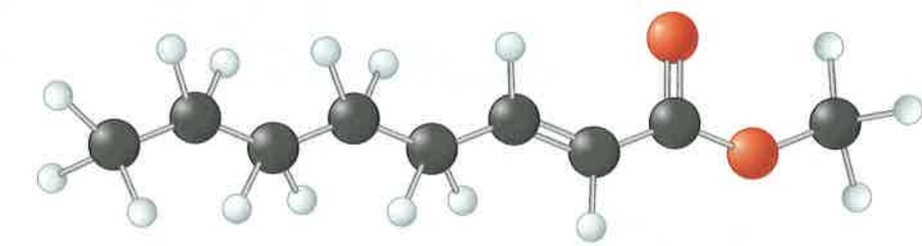
LESSON

12 What Shape Is That Smell?

Space-Filling Models

Think About It

Methyl octenoate, $C_9H_{16}O_2$, is a compound that smells like violets. A ball-and-stick model of methyl octenoate shows that it is a series of overlapping tetrahedral shapes stuck together. There is a trigonal planar segment in the area of the double bonds. But how would you describe the shape of the *whole* molecule? And does the shape of the whole molecule have anything to do with its smell?



How is the shape of a molecular compound related to its smell?

To answer this question, you will examine

1. Space-Filling Models
2. Relating Shape and Smell

SCILINKS NSTA
Topic: Molecular Modeling
Visit: www.SciLinks.org
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Exploring the Topic

1 Space-Filling Models

Most of the smell molecules you have encountered are considerably larger than three, four, or five atoms. The best way to look at the overall shape of these molecules is with a different type of model, called a **space-filling model.**

Take a moment to compare the ball-and-stick model of methyl octenoate with the space-filling model. In a space-filling model the sticks between atoms have been eliminated. There is no space between atoms. Instead, bonded atoms are shown slightly overlapping.

Methyl octenoate, $C_9H_{16}O_2$

Ball-and-stick model Space-filling model