Learning Objectives

• Determine the molecular mass of a molecule.
• Predict the general shape of a simple covalent molecule.

Unlike the ions in ionic compounds, which are arranged in lattices called crystals, molecules of covalent compounds exist as discrete units with a characteristic mass and a certain three-dimensional shape.

Molecular Mass

The mass of a molecule—the molecular mass (sometimes called the molecular weight)—is simply the sum of the masses of its atoms. As with formula masses, it is important that you keep track of the number of atoms of each element in the molecular formula to obtain the correct molecular mass.

Example \(\PageIndex{1}\)

What is the molecular mass of each covalent compound?

a. \(\text{H}_2\text{O}\)
b. \(\text{C}_6\text{H}_6\)
c. \(\text{NO}_2\)
d. \(\text{N}_2\text{O}_5\)

Solution

Use the masses of the atoms from the Table A4.

The molecular formula \(\text{H}_2\text{O}\) indicates that there are two hydrogen atoms and one oxygen atom in each molecule. Summing the masses of these atoms,

\[\begin{align*}
2 \text{H} & : 2 \times 1.01 = 2.02 \text{u} \\
1 \text{O} & : + 16.00 \text{u} \\
\text{Total} & : 18.02 \text{u}
\end{align*}\]

The molecular mass of \(\text{H}_2\text{O}\) is 18.02 u.

\[\begin{align*}
6 \text{C} & : 6 \times 12.01 = 72.06 \text{u} \\
6 \text{H} & : 6 \times 1.01 = + 6.06 \text{u} \\
\text{Total} & : 78.12 \text{u}
\end{align*}\]

The molecular mass of \(\text{C}_6\text{H}_6\) is 78.12 u.

1 \text{N} : 14.01 \text{u}
\[ \text{2 O: } 2 \times 16.00 = +32.00 \text{ u} \]
\[ \text{Total: } 46.01 \text{ u} \]

The molecular mass of NO\textsubscript{2} is 46.01 u.

\[ \text{2 N: } 2 \times 14.01 = 28.02 \text{ u} \]
\[ \text{5 O: } 5 \times 16.00 = +80.00 \text{ u} \]
\[ \text{Total: } 108.02 \text{ u} \]

The molecular mass of N\textsubscript{2}O\textsubscript{5} is 108.02 u.

Note that the two different nitrogen and oxygen compounds in these examples have different molecular masses.

Exercise \( \PageIndex{1} \)

What is the molecular mass of each covalent compound?

a. C\textsubscript{2}H\textsubscript{2}

b. CO

c. CO\textsubscript{2}

d. BF\textsubscript{3}

Molecular Shape: VSEPR Theory

Unlike ionic compounds, with their extended crystal lattices, covalent molecules are discrete units with specific three-dimensional shapes. The shape of a molecule is determined by the fact that covalent bonds, which are composed of negatively charged electrons, tend to repel one another. This concept is called the valence shell electron pair repulsion (VSEPR) theory. For example, the two covalent bonds in BeCl\textsubscript{2} stay as far from each other as possible, ending up 180° apart from each other. The result is a linear molecule:

\[
\begin{array}{c}
\text{Cl} \\
\text{Be} \\
\text{Cl}
\end{array}
\]

The three covalent bonds in BF\textsubscript{3} repel each other to form 120° angles in a plane, in a shape called trigonal planar:

\[
\begin{array}{c}
\text{F} \\
\text{B} \\
\text{F}
\end{array}
\]

The molecules BeCl\textsubscript{2} and BF\textsubscript{3} actually violate the octet rule; however, such exceptions are rare and will not be discussed in this text.
Note

Try sticking three toothpicks into a marshmallow or a gumdrop and see if you can find different positions where your “bonds” are farther apart than the planar 120° orientation.

The four covalent bonds in CCl₄ arrange themselves three dimensionally, pointing toward the corner of a tetrahedron and making bond angles of 109.5°:

![Carbon tetrachloride molecule](image)

Molecules with lone electron pairs around the central atom have a shape based on the position of the atoms, not the electron pairs. For example, NH₃ has one lone electron pair and three bonded electron pairs. These four electron pairs repel each other and adopt a tetrahedral arrangement:

![Ammonia molecule](image)

However, the shape of the molecule is described in terms of the positions of the atoms, not the lone electron pairs. Thus, NH₃ is said to have a pyramidal shape, not a tetrahedral one. Similarly, H₂O has two lone pairs of electrons around the central oxygen atom, in addition to the two bonded pairs:

![Water molecule](image)

Although the four electron pairs adopt a tetrahedral arrangement due to repulsion, the shape of the molecule is described by the positions of the atoms only. The shape of H₂O is bent.

In determining the shapes of molecules, it is useful to first determine the Lewis diagram for a molecule. The shapes of molecules with multiple bonds are determined by treating the multiple bonds as one bond. Thus, CH₂O has a shape similar to that of BF₃:

![Formaldehyde molecule](image)

Example \(\PageIndex{2}\)

Describe the shape of each molecule.

a. PCl₃
b. CO₂

Solution
a. The Lewis diagram for PCl₃ is as follows:

![Lewis diagram for PCl₃]

The four electron pairs arrange themselves tetrahedrally, but the lone electron pair is not considered in describing the molecular shape. Like NH₃, this molecule is pyramidal.

b. The Lewis diagram for CO₂ is as follows:

![Lewis diagram for CO₂]

The multiple bonds are treated as one group. Thus, CO₂ has only two groups of electrons that repel each other. They will direct themselves 180° apart from each other, so CO₂ molecules are linear.

Exercise \(\PageIndex{2}\))

Describe the shape of each molecule.

a. CBr₄
b. BCl₃

**Concept Review Exercises**

1. How do you determine the molecular mass of a covalent compound?
2. How do you determine the shape of a molecule?

**Answers**

1. The molecular mass is the sum of the masses of the atoms in the formula.
2. The shape of a molecule is determined by the position of the atoms, which in turn is determined by the repulsion of the bonded and lone electron pairs around the central atom.

**Key Takeaways**

- A molecule has a certain mass, called the molecular mass.
- Simple molecules have geometries that can be determined from VSEPR theory.
Exercises

1. What is the molecular mass of each compound?
   a. H₂S
   b. N₂O₄
   c. ICl₃
   d. HCl

2. What is the molecular mass of each compound?
   a. O₂F₂
   b. CCl₄
   c. C₆H₆
   d. SO₃

3. Aspirin (C₉H₈O₄) is a covalent compound. What is its molecular mass?

4. Cholesterol (C₂₇H₄₆O) is a biologically important compound. What is its molecular mass?

5. What is the shape of each molecule?
   a. H₂S
   b. COCl₂
   c. SO₂

6. What is the shape of each molecule?
   a. NBr₃
   b. SF₂
   c. SiH₄

7. Predict the shape of nitrous oxide (N₂O), which is used as an anesthetic. A nitrogen atom is in the center of this three-atom molecule.

8. Predict the shape of acetylene (C₂H₂), which has the two carbon atoms in the middle of the molecule with a triple bond. What generalization can you make about the shapes of molecules that have more than one central atom?

Answers

1. a. 34.62 u
   b. 92.02 u
   c. 233.25 u
   d. 36.46 u
3. 180.17 u

5. a. bent
   b. trigonal planar
   c. bent

7. bent

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