Pearson

4.3: Representing Compounds: Chemical Formulas and Molecular Models

The quickest and easiest way to represent a compound is with its **chemical formula**, which indicates the elements present in the compound and the relative number of atoms or ions of each. For example, H_2O is the chemical formula for water—it indicates that water consists of hydrogen and oxygen atoms in a two-to-one ratio. The formula contains the symbol for each element and a subscript indicating the relative number of atoms of the element. A subscript of 1 is typically omitted. Chemical formulas normally list the more metallic (or more positively charged) element first, followed by the less metallic (or more negatively charged) element. Examples of common chemical formulas include NaCl for sodium chloride, indicating sodium and chloride ions in a one-to-one ratio; CO_2 for carbon dioxide, indicating carbon and oxygen atoms in a one-to-two ratio; and CCl_4 for carbon tetrachloride, indicating carbon and chlorine in a one-to-four ratio.

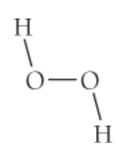
Types of Chemical Formulas

We categorize chemical formulas into three different types: empirical, molecular, and structural. An **empirical formula** indicates the *relative* number of atoms of each element in a compound. A **molecular formula** indicates the *actual* number of atoms of each element in a molecule of a compound. For example, the empirical formula for hydrogen peroxide is HO, but its molecular formula is H_2O_2. The molecular formula is always a whole-number multiple of the empirical formula. For some compounds, the empirical formula and the molecular formula are identical. For example, the empirical and molecular formula for water is H_2O because each water molecule contains two hydrogen atoms and one oxygen atom, and no simpler whole-number ratio can express the relative number of hydrogen atoms to oxygen atoms.

A **structural formula** uses lines to represent covalent bonds and shows how atoms in a molecule are connected or bonded to each other. The structural formula for H_2O_2 is:

H–O–O–H

Structural formulas can also indicate a sense of the molecule's geometry. The structural formula for hydrogen peroxide can also be written this way:



This version represents the approximate angles between bonds, giving a sense of the molecule's shape. Structural formulas can also depict the different types of bonds that occur within molecules. For example, consider the structural formula for carbon dioxide:

O=C=O

The two lines between each carbon and oxygen atom represent a double bond, which is generally stronger and shorter than a single bond (represented by a single line). A single bond corresponds to one shared electron pair, while a double bond corresponds to two shared electron pairs, as we will discuss in Section 4.7.

The type of formula we use depends on how much we know about the compound and how much we want to communicate. A structural formula communicates the most information, while an empirical formula communicates the least.

communicates the least.

Conceptual Connection 4.1 **Structural Formulas**

Example 4.1 Molecular and Empirical Formulas

Write the empirical formula for the compound represented by each molecular formula.

a. C_4H_8
b. B_2H_6
c. CCl_4

SOLUTION

To determine the empirical formula from a molecular formula, divide the subscripts by the greatest common factor (the largest number that divides exactly into all of the subscripts).

a. For C_4H_8, the greatest common factor is 4. The empirical formula is therefore CH_2.
b. For B_2H_6, the greatest common factor is 2. The empirical formula is therefore BH_3.
c. For CCl_4, the only common factor is 1, so the empirical formula and the molecular formula are the same.

FOR PRACTICE 4.1 Write the empirical formula for the compound represented by each molecular formula.

a. C_5H_{12}
b. Hg_2Cl_2
c. $C_2H_4O_2$

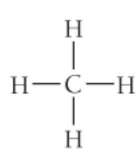
Molecular Models

A *molecular model* is a more accurate and complete way to specify a compound. A **ball-and-stick molecular model** represents atoms as balls and chemical bonds as sticks; how the two connect reflects a molecule's shape. The balls are typically color-coded to specific elements. For example, carbon is customarily black, hydrogen is white, nitrogen is blue, and oxygen is red. (For a complete list of colors of elements in the molecular models used in this book, see Appendix IIA.)

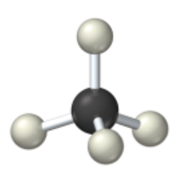
In a **space-filling molecular model**, atoms fill the space between each other to more closely represent best estimates for how a molecule might appear if scaled to visible size. Consider the following ways to represent a molecule of methane, the main component of natural gas:

CH_4

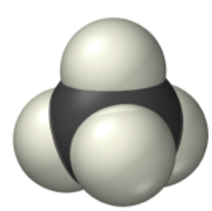
Molecular formula



Structural formula



Ball-and-stick model



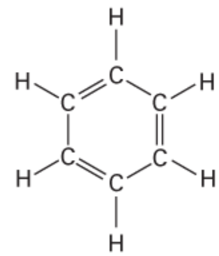
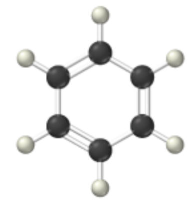
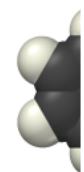
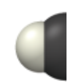
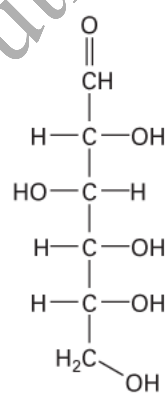
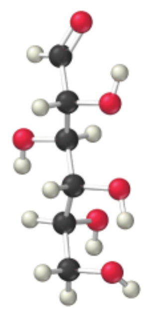
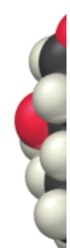
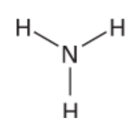
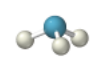
Space-filling model

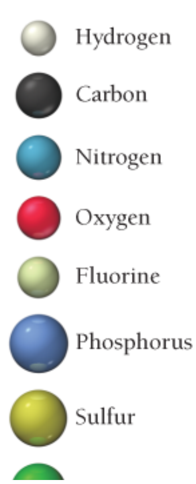
The molecular formula of methane indicates the number and type of each atom in the molecule: one carbon atom and four hydrogen atoms. The structural formula indicates how the atoms are connected: The carbon atom is bonded to the four hydrogen atoms. The ball-and-stick model clearly portrays the geometry of the molecule: The carbon atom sits in the center of a *tetrahedron* formed by the four hydrogen atoms. And finally, the space-

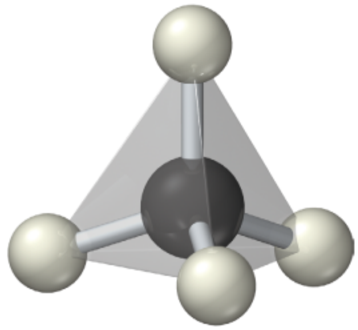
The carbon atom sits in the center of a *tetrahedron* formed by the four hydrogen atoms. And finally, the space filling model gives the best sense of the relative sizes of the atoms and how they merge together in bonding.

Throughout this book, you will see molecules represented in all of these ways. As you look at these representations, keep in mind what you learned in Chapter 1: The details about a molecule—the atoms that compose it, the lengths of the bonds between atoms, the angles of the bonds between atoms, and its overall shape—determine the properties of the substance that the molecule composes. Change any of these details and those properties change. Table 4.1 shows various compounds represented in the different ways we have just discussed.

Table 4.1 Benzene, Acetylene, Glucose, and Ammonia

Name of Compound	Empirical Formula	Molecular Formula	Structural Formula	Ball-and-Stick Model	Spac Mod
Benzene	CH	C_6H_6			
Acetylene	CH	C_2H_2	$H-C\equiv C-H$		
Glucose	CH_2O	$C_6H_{12}O_6$			
Ammonia	NH_3	NH_3			





A tetrahedron is a three-dimensional geometrical shape characterized by four equivalent triangular faces.

Conceptual Connection 4.2 **Representing Molecules**

Interactive