The Composition of Unknown Compounds

Are there signs of life on Mars? In 2008, NASA sent a robotic device called the *Phoenix Mars Lander* to the red planet to find out. The *Phoenix* searched Martian soil for water and for organic compounds that could only be produced by living things. Scientists equipped the *Phoenix* with a state-of-the-art analytical lab. A key component for this lab was a Thermal and Evolved Gas Analyzer (TEGA) (Figure 1). The TEGA consisted of a furnace connected to a mass spectrometer, which measures molecular masses.

In a typical analysis, the *Phoenix’s* robotic arm scooped samples of Martian soil into the TEGA’s furnace. Then the furnace temperature increased to vaporize any water or organic compounds present. The mass spectrometer “sniffed” the vapours to determine the molecular masses and concentrations of any compounds. Unfortunately, the TEGAs analyses showed no evidence of organic compounds; however, the *Phoenix* did find water!

**Combustion Analysis**

Chemists also use similar “burn and sniff” analytical tools to help identify unknown organic compounds on Earth (Figure 2). In this technology, a sample is burned with a plentiful oxygen supply, guaranteeing that complete combustion occurs. Any carbon dioxide and water produced during combustion is absorbed by chemicals in two successive chambers. Chemists use the change in the mass of these chambers to determine the mass of carbon dioxide and water produced. A mass spectrometer can also help to determine the molecular masses of the compounds.

**Percentage Composition**

We can determine the ratio of atoms or ions in a sample of a compound if we know the relative masses of its elements. With this information we can use the molar masses to convert from the relative masses to numbers of entities. Relative masses are usually given as percentage composition. **Percentage composition** is the percentage, by mass, of each element in the compound. Note that percentage composition is not the same as the ratios of atoms of elements.

**Table 1** shows the results of combustion analysis of an organic compound that contains the elements carbon, hydrogen, and oxygen. We can write the general formula for this compound as $C_xH_yO_z$. 

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*Figure 1* (a) A scientist in a “clean room” makes final adjustments to the Thermal and Evolved Gas Analyzer (TEGA) that the *Phoenix* used to detect water and organic compounds. (b) An artist’s impression shows the robotic arm of the *Phoenix* (lower left) about to take a soil sample.

*Figure 2* A combustion analysis apparatus is used to determine the composition of an unknown organic compound. The amounts of carbon dioxide and water produced in the analysis can be used to determine the percentage of carbon and hydrogen in the compound.
In Sample 1, for example, 0.801 g of the 2.00 g sample is carbon. The percentage of an element in a compound is determined using the equation

\[
\% \text{ element} = \frac{m_{\text{element}}}{m_{\text{sample}}} \times 100 \%
\]

Therefore the percentage of carbon in the compound is

\[
\% C = \frac{0.801 \text{ g}}{2.00 \text{ g}} \times 100 \% = 40.0 \%
\]

Repeating this calculation for the other elements and samples gives the percentages of carbon, hydrogen, and oxygen in the organic compound (Table 2).

Note that the percentages of carbon, hydrogen, and oxygen in this compound do not change regardless of the mass of the original compound. In fact, this result is valid for all chemical compounds and is known as the law of definite proportions.

### Law of Definite Proportions

The elements in a compound are always present in the same proportion by mass.

This law may seem obvious because we know that the number of atoms of each element in the compound is fixed. For example, the chemical formula H₂O states there are 2 hydrogen atoms and 1 oxygen atom in each molecule. Therefore, the proportion, by mass, of hydrogen to oxygen is always the same regardless of whether you pour a drop or a tubful of water (Figure 3).

However, the idea that a substance could have a fixed composition was met with considerable opposition when it was first proposed by the French chemist Joseph Proust in 1799. It only began to gain acceptance once John Dalton suggested that matter was composed of atoms in 1803.

### Tutorial 1 Calculating Percentage Composition

You can calculate percentage composition from either lab data or the chemical formula of the compound. We will analyze both of these situations.
Using Lab Data

The percentage of each element in a compound can be determined using the following formula:

\[
\% \text{ element} = \frac{m_{\text{element}}}{m_{\text{sample}}} \times 100\%
\]

- Note that both masses should have identical units. They need not both be in grams.
- Note also that mass units “cancel” as a result of division. Hence the answer has no units.

Sample Problem 1: Calculating Composition from Lab Data

A 500.00 mg tablet of Aspirin, C9H8O4, contains 300.00 mg carbon and 8.08 mg hydrogen. The remaining mass is oxygen. Determine the percentage composition of Aspirin.

Given: \(m_{\text{C,9H8O4}} = 500.00 \text{ mg}; \quad m_{\text{C}} = 300.00 \text{ mg}; \quad m_{\text{H}} = 8.08 \text{ mg}\)

Required: percentage composition of each element: \% C; \% H; \% O

Solution:

Step 1. Use the \% element formula, above, to calculate the percentage composition of each element for which you know the mass.

\[
\% \text{ C} = \frac{m_{\text{carbon}}}{m_{\text{sample}}} \times 100\% = \frac{300.00 \text{ mg}}{500.00 \text{ mg}} \times 100\% = 60.00\%
\]

\[
\% \text{ H} = \frac{m_{\text{hydrogen}}}{m_{\text{C,H,O_4}}} \times 100\% = \frac{8.08 \text{ mg}}{500.00 \text{ mg}} \times 100\% = 1.62\%
\]

Step 2. Determine the percentage of the element for which you do not know the mass by subtracting the sum of the percentages of the other elements from 100 \%. In this case, the remaining mass of the Aspirin tablet is oxygen. Therefore,

\[
\% \text{ O} = 100\% - (60.00\% + 1.62\%) = 100\% - (61.62\%) = 38.38\%
\]

Statement: The percentage composition of Aspirin is 60.00\% carbon, 1.62\% hydrogen, and 38.38\% oxygen.

Practice

1. Researchers have isolated a compound that contains only nitrogen and oxygen. They found that a 4.60 g sample of this compound contains 1.40 g of nitrogen. Find the percentage composition of this compound. \([\text{ans: } 30.4\% \text{ N}, 69.6\% \text{ O}]\)

2. A lab technician finds that an 11.5 g sample of a liquid compound contains 6.00 g of carbon and 1.51 g of hydrogen. The remaining mass is oxygen. Determine the percentage composition of this compound. \([\text{ans: } 52.2\% \text{ C}, 13.1\% \text{ H}, 34.7\% \text{ O}]\)

Using the Chemical Formula

Percentage composition has many applications in consumer products. Gardeners, for example, distinguish types of fertilizers by a three-number code (Figure 4). These numbers refer to the percentage of three nutrients in the product: nitrogen, phosphorus, and potassium.
When you are calculating percentage composition from a chemical formula, you calculate the contribution of each element toward the total mass. You will need to look up the atomic mass of each element and consider how many atoms there are in a molecule (or formula unit) of the compound. You can use either atomic mass units (u) or grams (g) as the units for mass, but remember to use the same unit for each element.

The molecular mass (or mass of one formula unit) of a compound has the same numerical value as its molar mass. Therefore, the atomic mass unit, u, or g/mol can be used in the percentage composition calculation. The atomic mass unit, u, is used in the following sample problem.

**Sample Problem 2: Calculating Composition from the Chemical Formula**

Determine the percentage composition of calcium hydroxide, Ca(OH)\(_2\).

**Given:** Ca(OH)\(_2\)

**Required:** percentage composition of Ca(OH)\(_2\)

**Solution:**

**Step 1.** Calculate the molecular mass of the compound.

\[ M_{\text{Ca(OH)}_2} = 74.10 \, \text{u} \]

**Step 2.** Calculate the percentage of each element by dividing the total mass of the element by the molecular mass and multiplying by 100%.

\[ \% \text{Ca} = \frac{40.08 \, \text{u}}{74.10 \, \text{u}} \times 100\% = 54.09\% \]

\[ \% \text{O} = \frac{32.00 \, \text{u}}{74.10 \, \text{u}} \times 100\% = 43.18\% \]

\[ \% \text{H} = \frac{2.02 \, \text{u}}{74.10 \, \text{u}} \times 100\% = 2.73\% \]

**Step 3.** Check that all the percentages add up to 100%.

54.09% + 43.18% + 2.73% = 100%

**Statement:** The percentage composition of calcium hydroxide is 54.09 % calcium, 43.18 % oxygen, and 2.73 % hydrogen.

**Practice**

3. Determine the percentage composition of each of the following compounds:

   (a) sodium sulfate, Na\(_2\)SO\(_4\)  
   [ans: (a) 32.37 % Na, 22.58 % S, 45.05 % O]

   (b) ammonium nitrate, NH\(_4\)NO\(_3\)  
   [ans: (b) 35.00 % N, 5.05 % H, 59.95 % O]

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**Percentage Composition of Alloys and Mixtures**

Alloys are mixtures of different metals blended together to form useful products. Unlike compounds, the percentage composition of an alloy can vary. For example, stainless steel used to make cutlery contains about 10 % chromium by mass. Surgical stainless steel contains at least 18 % chromium. Increasing the proportion of chromium makes steel more resistant to corrosion, a critical property for implants like knee replacements.

We can also consider the percentage composition of substances in mixtures. The food industry is often concerned about the water, salt, or fat content in their products.
### 6.6 Summary

- The percentage composition of a compound is the proportion of each element in the compound, by mass.
- Percentage composition can be found experimentally or from the chemical formula of the compound.
- The law of definite proportions states that a compound always has the same proportion of elements by mass. This occurs because the relative number of atoms or ions in the compound is fixed.

### 6.6 Questions

1. In a percentage composition investigation a compound was decomposed into its elements: 20.0 g of calcium, 6.0 g of carbon, and 24.0 g of oxygen. Determine the percentage composition of this compound.

2. A researcher performed a combustion analysis on a 5.00 g sample of ethanol, the alcohol in wine. The data showed that the sample contained 2.61 g of carbon and 0.66 g of hydrogen. The researcher assumed that the remaining mass was oxygen. Calculate the percentage composition of ethanol.

3. Hydrogen peroxide, $H_2O_2$, decomposes at room temperature to release oxygen gas. Use the law of definite proportions to explain why doubling the quantity of hydrogen peroxide doubles the quantity of oxygen produced.

4. (a) A lab analysis of a 10.00 g sample of benzene indicates that it contains 9.20 g of carbon. What is the mass of hydrogen in the sample? Explain.
   (b) What is the percentage composition of benzene?

5. Predict which compound in each of the following pairs has the greater percentage of carbon, by mass.
   (a) $C_2H_6$ or $C_2H_4$
   (b) $C_2H_6$ or $C_3H_6$
   (c) $C_2H_4$ or $C_3H_6$

6. Calcium oxide, $CaO$, is a key ingredient in cement. Calcium oxide is made by heating calcium carbonate, $CaCO_3$.
   \[ CaCO_3(s) \xrightarrow{heat} CaO(s) + CO_2(g) \]
   Explain what effect heat has on the following quantities:
   (a) the total mass of solids in the furnace
   (b) the percentage of calcium in the solids in the furnace

7. Calculate the percentage composition of the following compounds:
   (a) phosphoric acid, $H_3PO_4$ (gives pop a tart taste)
   (b) copper(I) sulfide, $Cu_2S$ (found in copper ore)
   (c) iron(III) oxide, $Fe_2O_3$ (a component in rust)
   (d) boric acid, $B(OH)_3$ (an antiseptic)

8. Ammonium phosphate, $(NH_4)_3PO_4$, and ammonium nitrate, $NH_4NO_3$, are both used in the production of fertilizers. Predict which compound contains the greater percentage of nitrogen. Verify your prediction by calculating the percentage of nitrogen in each compound.

9. Research, and prepare a short presentation on, gold fingerprinting.