GENERAL CHEMISTRY STANDARD 7.5

7.5: Identify a compound's empirical formula and calculate the molecular formula from the empirical formula and other data

DEFINITIONS

- **Empirical Formula:** The simplest, whole-number atom ratio of atoms in a formula
- **Molecular Formula:** The actual number of each type of atom that exists in one molecule of a substance
  - A compound's empirical formula can be determined using percent composition data
  - Additional data is needed to determine a compound's molecular formula

EXAMPLE

- Benzene is a dangerous organic compound. The molecular weight of benzene is 78 g/mol and it has a percent composition of 92.2% carbon and 7.8% hydrogen by mass. Find the empirical and molecular formulas of benzene.

First, assume a 100. g sample, resulting in 92.2 g of carbon and 7.8 g of hydrogen.

Next, convert these two masses to moles:

$$\frac{92.2 \text{ g C}}{} \left| \frac{1 \text{ mol C}}{12.00 \text{ g C}} \right. = 7.68 \text{ mol C}$$

$$\frac{7.8 \text{ g H}}{} \left| \frac{1 \text{ mol C}}{1.01 \text{ g H}} \right. = 7.72 \text{ mol H}$$

Now, divide the mole amounts out to determine the ratio:

7.68 / 7.72 ~ 1 So the empirical formula is CH

EXAMPLE CONTINUED

Now calculate the molecular weight of the empirical formula.

Carbon:	12.00 g	x 1 atom	12.00 g
Hydrogen:	1.01 g	x 1 atom	+ 1.01 g
			13.01 g

Now, divide the molecular weight of benzene by the molecular weight of the empirical formula:

78 g / 13.01 g = 5.995 ~ 6

So multiply each of the atoms in the empirical formula by six to get the molecular formula:

C_6H_6

EXAMPLE

- Glucose has a molecular weight of 180 g/mol and a percent composition of 40.0% carbon, 6.72% hydrogen, and 53.3% oxygen by mass. Determine the empirical and molecular formulas.

EXAMPLE

First, assume a 100. g sample, resulting in 40.0 g of carbon, 6.72 g hydrogen, and 53.3 g of oxygen.

Next, convert these three masses to moles:

53.3 g C	1 mol O	= 3.33 mol O
	15.99 g O	

40.0 g C	1 mol C	= 3.33 mol C
	12.00 g C	

6.72 g H	1 mol C	= 6.65 mol H
	1.01 g H	

Now, divide all mole amounts by the smallest mole amount, 3.33 mol in this case:
4.44 / 3.33 = 1.00 mol O
3.33 / 3.33 = 1.00 mol C
6.65 / 3.33 = 1.99 ~ 2 mol H

So the empirical formula is CH_2O

EXAMPLE CONTINUED

Now calculate the molecular weight of the empirical formula.

Carbon:	12.00 g	x 1 atom	12.00 g
Hydrogen:	1.01 g	x 2 atoms	2.02 g
Oxygen:	15.99 g	x 1 atom	+ 15.99 g
			30.01 g

Now, divide the molecular weight of glucose by the molecular weight of the empirical formula:

180 g / 30.01 g = 5.998 ~ 6

So multiply each of the atoms in the empirical formula by six to get the molecular formula:

$C_6H_{12}O_6$