CHEMICAL QUANTITIES

Chapter Six

Introducing the Mole

- The dozen is a unit of quantity
  - If I have a dozen atoms, I have 12 atoms by definition.
- The <u>mole</u>(mol) is a very important unit of quantity in chemistry. It is used to count large numbers of atoms, molecules, and other submicroscopic pieces of matter.
- <u>If you have 1 mole of something, you have 6.022×10^{23} of it.</u>

Examples

- How many eggs are in 5.5 dozen eggs?
- How many helium atoms are in 1.55 moles of helium?
  - Why do we use dozen for eggs and moles for atoms?

Atomic Weights and The Mole

- The atomic weights provided on the periodic table can be used in much more convenient units than amu.
- The values on the periodic table can be interpreted as grams per mole of the atom.
  - For example, 1 mol of calcium atoms has a mass of 40.08 g; 1 mol of neon atoms has a mass of 20.18 g.
- Note that atomic weights are often also called <u>molar masses.</u>

Practice Using the Mole

Examples:

1. What is the mass (in grams) of 0.558 moles of zinc?

2. How many atoms are contained in 425. grams of pure silver?

3. The density of aluminum is 2.702 g/cm^3. How many atoms are there in a sphere of pure aluminum with radius 2.25 cm?

Molecular Weights

- The mass of molecules can be calculated by adding up the atomic weights of the individual atoms making up the molecule.
- For example, suppose we wanted to know the molecular weight of CO_2.
  - Every 1 mol of CO_2 contains_____mole of C atoms and_____moles of O atoms.
  - Calculate the total mass of all of these atoms and add them up to get the molecular weight of CO_2.
  - Aside: what is the mass of a single molecule of CO_2 in amu?
- Note that the term *formula weight* is applied for those compounds which do not form true molecules (ionic compounds like NaCl and CaO).

Examples

- Determine the molecular weights of glucose ($C_6H_{12}O_6$) and acetic acid (CH_3CO_2H).

Percent Composition

- One common technique used in specialized chemical laboratories is elemental analysis, which can be used to determine the percent each element in a compound contributes to its mass.
- Since this type of data is very common, it is important that we know how to interpret it and put it to practical use.

Percent Composition

- The percent composition is the percent of the total mass percent of each element in a compound.
- To determine its value, we use the following formula for each element in the compound:

$$\% \text{ composition} = \frac{\text{total mass of element}}{\text{molar mass}} \times 100\%$$

Example

What is the percent composition of each element in acetic acid?

Example

Percent compositions can also be determined for mixtures, such as alloys.

Suppose that 5.50 mols each of copper and zinc are blended with 2.43 mols of tin to make an alloy. What is the percent composition of the alloy?

$5.50 + 5.50 + 2.43 = 13.43$ total moles

Cu: $(5.50/13.43) * 100 = 41.0\%$

Zn: $(5.50/13.43) * 100 = 41.0\%$

Sn: $(2.43/13.43) * 100 = 18.0\%$

Example

- A 19.82 g chunk of an ore is analyzed and found to have a percent composition of 5.75% silver, 64.33% iron, and the remainder is silicon. What mass of each element is contained in a 4.87 kg sample of this ore?

One Last Example

A student determines the mass of a hydrate sample to be 6.873 g. After strongly heating the sample for 20 minutes to remove water, he reweighs the sample, finding the mass to be 5.276 g. What percent of the mass of the original hydrate is water?

6.873g – 5.276g = 1.597g lost

*(1.597g/6.873g)*100 = 23.24% is water and 76.76% is the compound.*

Molecular and Empirical Formulas

- The molecular formula of a compound tells us exactly how many atoms of each element are contained in a compound.
- In contrast, the empirical formula only tells us the lowest whole-number ratio between each element
- For example, glucose has molecular formula $C_6H_{12}O_6$ (each molecule of glucose contains 6 carbon atoms, 12 hydrogen atoms, and 6 oxygen atoms)
- Glucose then has empirical formula CH_2O (1 C to 2 H to 1 O is the lowest whole-number ratio).

Empirical Formulas

- While the molecular formula ultimately is more useful for most applications, it is often more difficult to determine than the empirical formula.
- When a sample is analyzed we can easily determine the percent composition, and from here find the ratio of the number of atoms of each element.
- Information on the exact number of atoms in each molecule cannot be found in this way.

Determining the Empirical Formula

- A simple series of steps can be used to determine the empirical formula of a compound:
  - Find the mass of each element in the compound
  - Convert the masses into moles of each element
  - Express the moles of atoms as the smallest possible whole-number ratio
  - Use the numbers from these ratios in the empirical formula for each element.

Empirical Formulas

- The simplest, whole-number ratio of atoms in a molecule is called the **empirical formula**.
  - Can be determined from percent composition or combining masses.
- The molecular formula is a multiple of the empirical formula.

$$\%\ A \xrightarrow{100g} \text{mass A (g)} \xrightarrow{MM_A} \text{moles A}$$

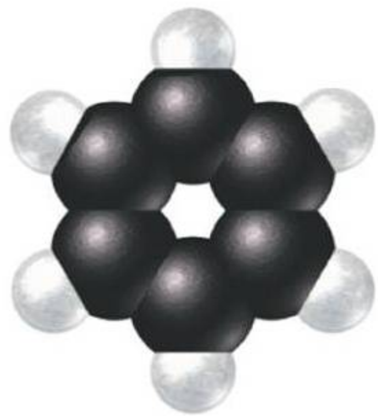
$$\%\ B \xrightarrow{100g} \text{mass B (g)} \xrightarrow{MM_B} \text{moles B}$$

$$\longrightarrow \frac{\text{moles A}}{\text{moles B}}$$

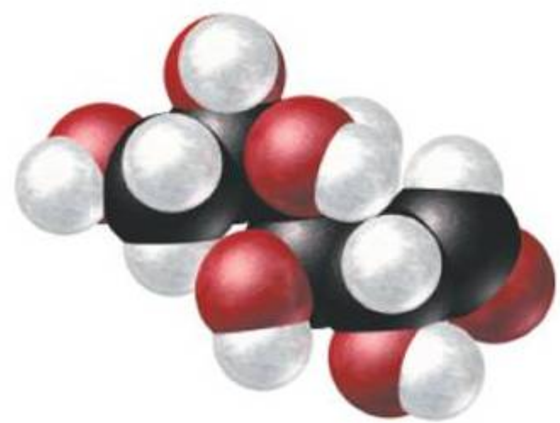
Empirical Formulas, Continued

Hydrogen Peroxide
Molecular formula = H_2O_2
Empirical formula = HO

Benzene
Molecular formula = C_6H_6
Empirical formula = CH



Glucose
Molecular formula = $C_6H_{12}O_6$
Empirical formula = CH_2O



Practice—Determine the Empirical Formula of Benzopyrene, $C_{20}H_{12}$, Continued

- Find the greatest common factor (GCF) of the subscripts.

  20 factors = (10 x 2), (5 x 4)

  12 factors = (6 x 2), (4 x 3)

  GCF = 4

- Divide each subscript by the GCF to get the empirical formula.

  $C_{20}H_{12} = (C_5H_3)_4$

  Empirical formula = C_5H_3

Finding an Empirical Formula

1. Convert the percentages to grams.
   a. Skip if already grams.
2. Convert grams to moles.
   a. Use molar mass of each element.
3. Write a pseudoformula using moles as subscripts.
4. Divide all by smallest number of moles.
5. Multiply all mole ratios by number to make all whole numbers, if necessary.
   a. If ratio ?.5, multiply all by 2; if ratio ?.33 or ?.67, multiply all by 3, etc.
   b. Skip if already whole numbers after Step 4.

Example:

- A laboratory analysis of aspirin determined the following mass percent composition. Find the empirical formula.

$$C = 60.00\%$$

$$H = 4.48\%$$

$$O = 35.53\%$$

Example: Find the empirical formula of aspirin with the given mass percent composition.

- Write down the given quantity and its units.

Given: C = 60.00%

H = 4.48%

O = 35.53%

Therefore, in 100 g of aspirin there are 60.00 g C, 4.48 g H, and 35.53 g O.

Example: Find the empirical formula of aspirin with the given mass percent composition.	Information: Given: 60.00 g C, 4.48 g H, 35.53 g O

- Write down the quantity to find and/or its units.

  Find: empirical formula, $C_xH_yO_z$

Example:
Find the empirical formula of aspirin with the given mass percent composition.

Information:

Given: 60.00 g C, 4.48 g H, 35.53 g O

Find: empirical formula, $C_xH_yO_z$

- Collect needed conversion factors:

$$1 \text{ mole C} = 12.01 \text{ g C}$$

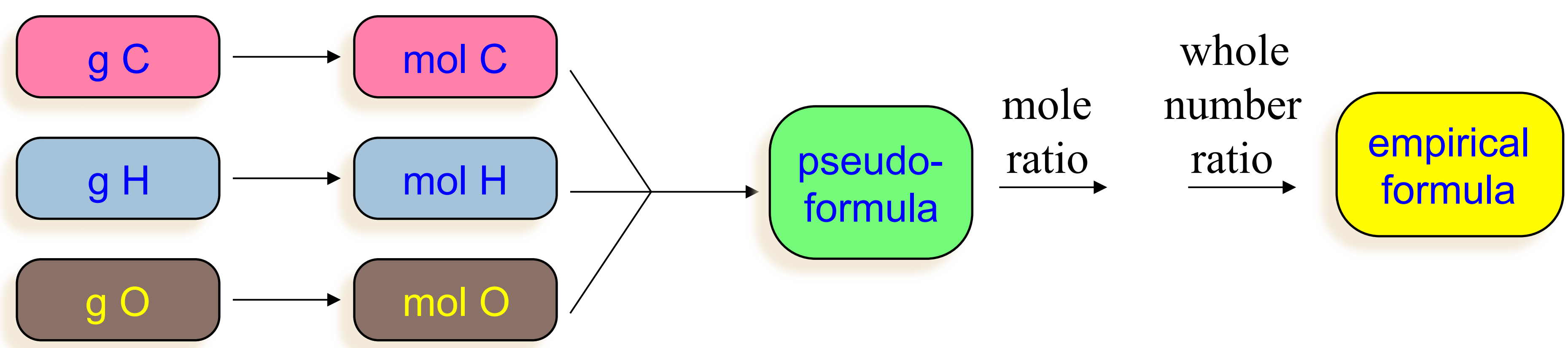
$$1 \text{ mole H} = 1.01 \text{ g H}$$

$$1 \text{ mole O} = 16.00 \text{ g O}$$

Example:
Find the empirical formula of aspirin with the given mass percent composition.

Information:
Given: 60.00 g C, 4.48 g H, 35.53 g O
Find: empirical formula, $C_xH_yO_z$
Conversion Factors:
1 mol C = 12.01 g; 1 mol H = 1.01 g;
1 mol O = 16.00 g

- Write a solution map:



Example:
Find the empirical formula of aspirin with the given mass percent composition.

Information:

Given: 60.00 g C, 4.48 g H, 35.53 g O

Find: empirical formula, $C_xH_yO_z$

Conversion Factors:

1 mol C = 12.01 g;
1 mol H = 1.01 g; 1 mol O = 16.00 g

Solution Map: g C,H,O → mol C,H,O → mol ratio → empirical formula

- Apply the solution map:
  - Calculate the moles of each element.

$$60.00\,\cancel{\text{g C}} \times \frac{1\,\text{mol C}}{12.01\,\cancel{\text{g C}}} = 4.996\,\text{mol C}$$

$$4.48\,\cancel{\text{g H}} \times \frac{1\,\text{mol H}}{1.01\,\cancel{\text{g H}}} = 4.44\,\text{mol H}$$

$$35.53\,\cancel{\text{g O}} \times \frac{1\,\text{mol O}}{16.00\,\cancel{\text{g O}}} = 2.221\,\text{mol O}$$

Example:
Find the empirical formula of aspirin with the given mass percent composition.

Information:

Given: 4.996 mol C, 4.44 mol H, 2.221 mol O

Find: empirical formula, $C_xH_yO_z$

Conversion Factors:

1 mol C = 12.01 g;
1 mol H = 1.01 g; 1 mol O = 16.00 g

Solution Map: g C,H,O → mol C,H,O → mol ratio → empirical formula

- Apply the solution map:
  - Write a pseudoformula.

$$C_{4.996}H_{4.44}O_{2.221}$$

Example:
Find the empirical formula of aspirin with the given mass percent composition.

Information:

Given: $C_{4.996}H_{4.44}O_{2.221}$

Find: empirical formula, $C_xH_yO_z$

Conversion Factors:

1 mol C = 12.01 g;
1 mol H = 1.01 g; 1 mol O = 16.00 g

Solution Map: g C,H,O → mol C,H,O → mol ratio → empirical formula

- Apply the solution map:
  - Find the mole ratio by dividing by the smallest number of moles.

$$C_{\frac{4.996}{2.221}}H_{\frac{4.44}{2.221}}O_{\frac{2.221}{2.221}}$$

$$C_{2.25}H_2O_1$$

Example:
Find the empirical formula of aspirin with the given mass percent composition.

Information:

Given: $C_{2.25}H_2O_1$

Find: empirical formula, $C_xH_yO_z$

Conversion Factors:

1 mol C = 12.01 g;
1 mol H = 1.01 g; 1 mol O = 16.00 g

Solution Map: g C,H,O → mol C,H,O → mol ratio → empirical formula

- Apply the solution map:
  - Multiply subscripts by factor to give whole number.

$$\{C_{2.25}H_2O_1\} \times 4$$

$$C_9H_8O_4$$

Example

A sample of a compound is analyzed, and found to contain 1.61 g of phosphorus and 2.98 g of fluorine. What is the empirical formula of this compound?

1.61g P * (1 mole P/30.97 g) = 0.051986 moles P

2.98 g F * (1 mole F/19.00 g) = 0.156842 moles F

P: (0.051986/0.051986) = 1

F: (0.156842/0.051986) = 3

Empirical Formula = PF_3

Example

The mass of a piece of iron is 1.62 g. The iron is exposed to oxygen and reacts to form a pure oxide of iron, now with mass of 2.31 g. What is the empirical formula of this oxide?

1.62 g Fe * (1 mole Fe/55.85 g) = 0.02901 moles Fe

2.31 g – 1.62 g = 0.69 g of O

0.69 g of O * (1 mole/15.99 g) = 0.043152 moles

Fe: 0.02901/0.02901 = 1

O: 0.043152/0.02901 = 1.4875

$FeO_{1.4875}$ x 2 = $\mathbf{Fe_2O_3}$

Molecular Formula

- Given the empirical formula and the molecular weight of a compound, it is possible to determine the molecular formula.
- For example, suppose we have a compound with empirical formula CH.
  - Its molecular formula could be CH, C_2H_2, C_3H_3, etc.
- Now, let's see what the formula weight would be for each:

Molecular Formula

- $CH = 13.02$ g/mol
- $C_2H_2 = 26.04$ g/mol
- $C_3H_3 = 39.06$ g/mol
- Notice that each is a multiple of 13.02!

- To determine the molecular formula from this information
  - Find the formula weight of the empirical formula
  - Divide the molecular weight by this value (you should get a whole number).
  - Multiply the subscripts in your empirical formula by this whole number.
- You now have your molecular formula.

All These Molecules Have the Same Empirical Formula. How Are the Molecules Different?

Name	Molecular Formula	Empirical Formula	
Glyceraldehyde	$C_3H_6O_3$	CH_2O	
Erythrose	$C_4H_8O_4$	CH_2O	
Arabinose	$C_5H_{10}O_5$	CH_2O	
Glucose	$C_6H_{12}O_6$	CH_2O	

All These Molecules Have the Same Empirical Formula. How Are the Molecules Different?, Continued

Name	**Molecular Formula**	**Empirical Formula**	**Molar Mass, g**
Glyceraldehyde	$C_3H_6O_3$	CH_2O	90
Erythrose	$C_4H_8O_4$	CH_2O	120
Arabinose	$C_5H_{10}O_5$	CH_2O	150
Glucose	$C_6H_{12}O_6$	CH_2O	180

Molecular Formulas

- The molecular formula is a multiple of the empirical formula.
- To determine the molecular formula, you need to know the empirical formula and the molar mass of the compound.

$$\frac{\text{Molar mass}_{\text{real formula}}}{\text{Molar mass}_{\text{empirical formula}}} = \text{Factor used to multiply subscripts}$$

Example—Determine the Molecular Formula of Cadinene if it has a Molar Mass of 204 g and an Empirical Formula of C_5H_8.

1. Determine the empirical formula.
   - May need to calculate it as previous.

$$C_5H_8$$

2. Determine the molar mass of the empirical formula.

$$5\ C = 60.05,\ 8\ H = 8.064$$

$$C_5H_8 = 68.11\ g/mol$$

Example—Determine the Molecular Formula of Cadinene if it has a Molar Mass of 204 g and an Empirical Formula of C_5H_8, Continued.

3. Divide the given molar mass of the compound by the molar mass of the empirical formula.
   - Round to the nearest whole number.

$$\frac{204\ \cancel{\text{g/mol}}}{68.11\ \cancel{\text{g/mol}}} = 3$$

Example—Determine the Molecular Formula of Cadinene if it has a Molar Mass of 204 g and an Empirical Formula of C_5H_8, Continued.

4. Multiply the empirical formula by the factor above to give the molecular formula.

$$(C_5H_8)_3 = C_{15}H_{24}$$

Practice—Benzopyrene has a Molar Mass of 252 g and an Empirical Formula of C_5H_3. What is its Molecular Formula? (C = 12.01, H=1.01)

Practice—Benzopyrene has a Molar Mass of 252 g and an Empirical Formula of C_5H_3. What is its Molecular Formula? (C = 12.01, H=1.01), Continued

$$\begin{array}{llr} C_5 = & 5(12.01\text{ g}) = & 60.05\text{ g} \\ \underline{H_3 =} & \underline{3(1.01\text{ g}) =} & \underline{3.03\text{ g}} \\ C_5H_3 & = & 63.08\text{ g} \end{array}$$

$$n = \frac{252\ \cancel{\text{g/mol}}}{63.08\ \cancel{\text{g/mol}}} = 4$$

Molecular formula = $\{C_5H_3\}$ x 4 = $C_{20}H_{12}$

Practice—Determine the Molecular Formula of Nicotine, which has a Molar Mass of 162 g and is 74.0% C, 8.7% H, and the Rest N. (C=12.01, H=1.01, N=14.01)

Practice—Determine the Molecular Formula of Nicotine, which has a Molar Mass of 162 g and is 74.0% C, 8.7% H, and the Rest N, Continued

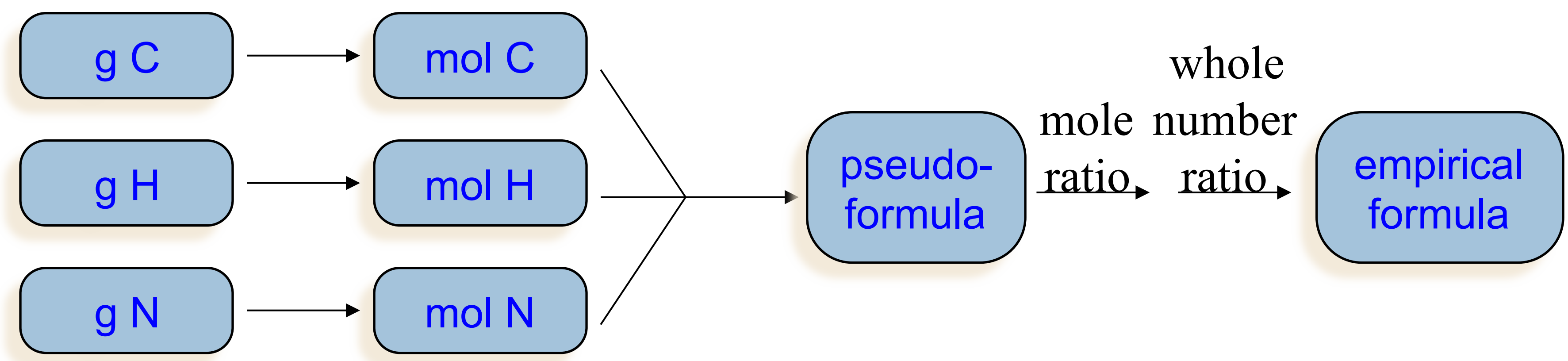
Given: 74.0% C, 8.7% H, {100 – (74.0+8.7)} = 17.3% N ∴
in 100 g nicotine there are 74.0 g C, 8.7 g H, and 17.3 g N.

Find: $C_xH_yN_z$

Conversion Factors:

1 mol C = 12.01 g; 1 mol H = 1.01 g; 1 mol N = 14.01 g

Solution Map:



Practice—Determine the Molecular Formula of Nicotine, which has a Molar Mass of 162 g and is 74.0% C, 8.7% H, and the Rest N, Continued.

Apply solution map:

$$74.0\,\cancel{g}\,C \times \frac{1\,mol\,C}{12.01\,\cancel{g}} = 6.16\,mol\,C$$

$$8.7\,\cancel{g}\,H \times \frac{1\,mol\,H}{1.01\,\cancel{g}} = 8.6\,mol\,H$$

$$17.3\,\cancel{g}\,N \times \frac{1\,mol\,N}{14.01\,\cancel{g}} = 1.23\,mol\,N$$

$$C_{6.16}H_{8.6}N_{1.23}$$

$$C_{\frac{6.16}{1.23}}H_{\frac{8.6}{1.23}}N_{\frac{1.23}{1.23}} = C_5H_7N$$

$C_5 =$	$5(12.01\ g) =$	$60.05\ g$
$N_1 =$	$1(14.01\ g) =$	$14.01\ g$
$H_7 =$	$7(1.01\ g) =$	$7.07\ g$
C_5H_7N	$=$	$81.13\ g$

$$\frac{\text{mol. mass nicotine}}{\text{mol. mass emp. form.}} = \frac{162\,\cancel{g}}{81.13\,\cancel{g}} = 2$$

$$\{C_5H_7N\} \times 2 = C_{10}H_{14}N_2$$