Chapter 3: Molecular analysis

Read: BLB 2.6, 3.3–3.5
HW: BLB 3:21a, c, e, f, 25, 29, 37, 49, 51, 53
Packet 3:1–8

Know:
• molecular & empirical formulas
• formula & molecular weights

No Score from Exam 1?
Go to 210 Whitmore and speak with Mike Joyce to get it straightened out.

Which Skill Check Test Bonus Deadline is Approaching?? ______________________

When is EXAM 2???
_______________________________

CHEMICAL FORMULA
• Formula that gives the TOTAL number of elements in a molecule or formula unit.

COEFFICIENTS AND SUBSCRIPTS

3O₂
2O₃

❖ Changing the coefficient changes the__________ of that molecule, not the identity.
❖ Changing the subscripts changes the__________ of the molecule.
Types of Chemical Formulas

MOLECULAR FORMULA
Chemical formula with subscripts of the total number of atoms in each molecule.

\[ \text{H}_2\text{O} \quad \text{H}_2\text{O}_2 \quad \text{O}_2 \quad \text{CH}_3\text{CH}_2\text{OH} \]

EMPIRICAL FORMULA
Chemical formula with the smallest integer subscripts for a given composition.

STRUCTURAL FORMULA
Chemical formula with structural information about connectivity and angles.

Connecting microscopic (atoms) to macroscopic (weight)

Use Formula Weight (Molar Mass or Molecular Weight)

- Definition:

  - water
  - methanol
  - nickel(II) perchlorate
Important Connections

• Formula weight

• Avagadro’s number

• Coefficient

• Subscript

• Empirical Formula

• Mass Percent

Working With Formulas

• How many atoms are in the formula \( \text{Mg}_3(\text{PO}_4)_2 \)?
  a) 3
  b) 5
  c) 10
  d) 13

• How many moles of \( \text{Mg}_3(\text{PO}_4)_2 \) are in a 10.0 g sample?
  a) 0.0380 moles
  b) 0.0595 moles
  c) 0.0431 moles

• How many atoms are in 10.0 g of \( \text{Mg}_3(\text{PO}_4)_2 \)?
  a) \( 2.59 \times 10^{22} \) atoms
  b) \( 3.58 \times 10^{22} \) atoms
  c) \( 2.29 \times 10^{22} \) atoms
  d) \( 2.97 \times 10^{23} \) atoms
Experimental Data often provides only the **Empirical Formula**

How do we find the molecular formula from experimental data?

### Percent Composition

**Connecting:**

*Empirical formula (lowest ratio) to Molecular formula (ratio in molecule)*

\[
\% \text{ of element} = \frac{(\text{atoms of element})(\text{AW})}{\text{FW of compound}} \times 100
\]

**OR, If we have 100 g of sample,**

\[
\% \text{ of element} = \frac{\text{mass of element}}{100 \text{ g sample}} \times 100
\]

**Note:** percentages must add up to 100%.
Working with mass percent

1. What is the mass percent of C in CO₂?

C = 12.01 amu  O = 16.0 amu

FW = 12.01 + 2(16.0) = 44.01 amu

2. I have 2g of a sample that is 54.2% C by mass. How many grams of C are in the sample?

STRATEGY:
If % C in an unknown substance is 54.2%, a 100g sample of that substance contains 54.2g of C.

Alternately: 0.542 is the fraction of the sample that contains carbon.

Now we can connect Empirical Formula to Mass Percent of Elements

Given one quantity, we can calculate the other:

- Start with mass % of elements (i.e. empirical data) and calculate a formula
- Start with the formula and calculate the mass % elements

Given:
- Mass % elements
  - Assume 100 g sample
  - Use atomic weights

Find:
- Empirical formula
  - Calculate mole ratio
  - Moles of each element
Sample Problem

- An analysis of nicotine, a poisonous compound found in tobacco leaves, shows that it is 74.0% C, 8.65% H and 17.35% N. Its molar mass is 162 g/mol. What are the empirical and molecular formulas of nicotine?

Empirical Formulas from Combustion Analysis

Problem Solving Strategy:
1. What do we need to find the empirical formula?
2. We have g CO₂ and g H₂O. How can we calculate the ratio of moles C atoms to moles H atoms?
3. Oxygen is in excess, and other elements are not analyzed for. We know the total mass of the sample. How can we find the mass of elements other than C and H in the molecule?
4. How can we calculate moles from mass?
5. What is the empirical formula?
Sample Combustion Analysis

1. A 4 g sample of an alcohol produces 7.65 g of CO₂ and 4.70 g of H₂O upon combustion. What is the empirical formula of the alcohol?

Working with balanced reactions; Stoichiometry

2C₈H₁₈ + 25O₂ → 16CO₂ + 18H₂O

• Energy is conserved

• Mass is conserved

• Stoichiometry
  Coefficients are the ratio of __________ of reactant to _____________ of product
To connect mass to moles, make a table:
Note Connections!

Balanced Combustion Reaction:
\[ 2C_8H_{18} + 25O_2 \rightarrow 16CO_2 + 18H_2O \]

Conservation of mass: Use Formula Weights

<table>
<thead>
<tr>
<th>Formula</th>
<th>Weight (g/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>12.01</td>
</tr>
<tr>
<td>H</td>
<td>1.01</td>
</tr>
<tr>
<td>O</td>
<td>15.99</td>
</tr>
<tr>
<td></td>
<td>18.02</td>
</tr>
</tbody>
</table>

Moles:

Molecules:

Atoms:

Stoichiometric Problem Solving

If a clean-burning engine burns 1 gallon of gasoline (assume it is pure octane, density 0.692 g/mL, and there are 3.7854 L in a gallon.), how many kg of CO\(_2\) will it produce?

1. What is the balanced chemical reaction?
\[ 2C_8H_{18} + 25O_2 \rightarrow 16CO_2 + 18H_2O \]

2. What do we know?
   a)

3. What do we need to find?
   a) Mass octane
   b) Moles octane
   c) Moles of CO\(_2\)
   d) Mass of CO\(_2\)
Stoichiometry Review

• Coefficients vs. Subscripts
• Covert
  
  mass → moles → molecules → atoms
• Calculate Empirical Formula given Mass %
  
  Assume 100 g sample;
  mass % atom = g atom
  
  Find moles of each atom
  Find ratio (divide by smallest)

Stoichiometry Review

• Calculate Molecular Formula from Empirical Formula
  
  Compare FW of sample to FW of empirical formula
  
  What integer relates them to each other?
  
  Multiply each atom in the empirical formula by that integer.
• Chemical Formulas
  - What do subscripts mean?
  - How is this different from a coefficient in a chemical reaction?
  - Calculate the number of atoms in a molecule.
  - What is a molecular formula?
  - What is a structural formula?
  - What is an empirical formula?
  - How is it related to the molecular formula?
  - Why is an empirical formula important?

• Molecular Weight
  - What is atomic weight?
  - What is molecular weight or formula weight (FW)?
  - How can you calculate FW of a given molecule using the periodic table?
  - Use the molecular weight to convert the mass of a sample into moles of molecules.
  - Use the molecular weight to convert moles into mass of molecules.
  - Convert moles of molecules into number of atoms using Avogadro’s number.
Percent Composition, Mass %

- Calculate mass percent of an element in a molecule; know the ratio you must use.
- Convert mass percent to grams, assuming you have 100 g of sample.
- Given the weight of a sample, use the mass percent to calculate the mass of an element in the sample.
- Given the mass percent, convert this to number of moles of each element in the sample, assuming 100 g of sample.

Empirical and Molecular Formula

- Given percentages of elements in a sample, determine the empirical formula using mole ratios.
- Given the FW of a compound, convert the empirical formula to the molecular formula. Find the integer that relates the two formulas.
• Combustion Analysis
  - Given the mass of CO$_2$ and H$_2$O produced, find the number of moles of C and moles of H in the original sample.
  - Find the mole ratio of C:H.
  - If another element is present (like O or N), find the moles of that element in the original sample by:
    • Calculating the mass of C and mass of H in the original sample using the number of moles and atomic weight.
    • Subtract the mass of C and the mass of H from the weight of the original sample to get mass of the extra element.
    • Convert mass of the extra element to moles, and find the mole ratio compared to the moles of C and H.
  - Write the empirical formula using the ratios.
  - Write the molecular formula if given the molecular weight of the original compound.

Stoichiometry Review

- Combustion Analysis
  - given g of CO$_2$ and H$_2$O produced
  - excess O$_2$
  - may have N or O in formula (non-C,H atoms)

Method
1. find moles of C and H atoms
2. Get ratio of C and H atoms
3. Find mass of C and H atoms
4. $\text{Mass}_{\text{sample}} - \text{Mass}_C - \text{Mass}_H = \text{Mass}_{\text{non-C,H atoms}}$
5. Find moles of non-C,H atoms, find ratio
6. Write empirical formula using ratios.
7. Convert to molecular formula if given sample FW.