Learning Objectives

- Use chemical formulas to solve various kinds of chemical problems
- Relate names to formulas and charges of simple ions
- Combine simple ions to write formulas and name simple ionic compounds
- Recognize and use formula weights and mole relations
- Interconvert masses, moles, and formulas
- Determine percent composition in compounds
- Determine formulas from composition data
- Recognize models from calculated molecular formulas
- Perform calculations of purity of substances

Chemical Formulas and Stoichiometry

Atoms, Particles & Molecules

- An atom is the smallest particle of an element that maintains its chemical identity.
- A molecule is the smallest particle of an element or a compound with a stable existence.
Atoms, Particles & Molecules

• Fundamental Particles
  • electron
  • proton
  • neutron
• Atoms contain equal numbers of electrons and protons

Atoms, Particles & Molecules

• The atomic number (Z) is the number of protons in the nucleus.

Chemical Formula

• Shows chemical composition.
• Represents elements present as whole-number ratio [most of the time]

Law of Definite Proportions

• The law of definite proportions states that a chemical compound always contains exactly the same proportion of elements by mass.
• An equivalent statement is the law of constant composition, which states that all samples of a given chemical compound have the same elemental composition.
• When water is separated into its component parts, the volume of hydrogen produced is twice as great as the volume of oxygen.

\[
\begin{array}{c|c|c}
\text{hydrogen} & \text{oxygen} \\
\text{H}_2 & \text{O} \\
\text{composition by volume} & 2 \text{ units} & 1 \text{ unit} \\
\text{composition by mass} & 11.11\% & 88.89\%
\end{array}
\]
Molecular Formula

- Formula for glycine is $\text{C}_2\text{H}_5\text{NO}_2$.
- In one molecule there are:
  - 2 C atoms
  - 5 H atoms
  - 1 N atom
  - 2 O atoms

Can also write glycine formula as $\text{H}_2\text{NCH}_2\text{COOH}$ to show atom ordering.

or in the form of a structural formula:

```
H  H  O
\ /
H-N-C-C-O-H
|  \H
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Elements That Exist As Molecules

Allotropes of C

- Diamond
- Buckyball, $\text{C}_{60}$
- Graphite

Allotropes of O

- allotropes are different forms of an element with the same state.

Ions and Ionic Compounds

- Ions are atoms or groups of atoms with a positive or negative charge.
- Taking away an electron from an atom gives a cation with a positive charge.
- Adding an electron to an atom gives an anion with a negative charge.

Stoichiometry

- Stoichiometry is the relationship between the relative quantities of substances taking part in a reaction or forming a compound, typically a ratio of whole integers.
Counting Atoms

• Chemistry is a quantitative science - we need a "counting unit."
• The MOLE
• 1 mole is the amount of substance that contains as many particles (atoms, molecules) as there are in 12.0 g of $^{12}$C.

Particles in a Mole

Avogadro's Number

$6.022145 \times 10^{23}$

Amedeo Avogadro
1776-1856

There are Avogadro's number of particles in a mole of any substance.

Atomic Weight

• Weighted average of the masses of the constituent isotopes of an element.
• Tells us the atomic masses of every known element.
• Lower number on periodic chart.
• How do we know what the values of these numbers are?

The Mole

• How do we know when we have a mole?
  • count it out
  • weigh it out
• Molar mass - mass in grams numerically equal to the atomic weight of the element in grams.
• H has an atomic weight of 1.00794 g
  • 1.00794 g of H atoms = $6.022 \times 10^{23}$ H atoms
• Mg has an atomic weight of 24.305 g
  • 24.305 g of Mg atoms = $6.022 \times 10^{23}$ Mg atoms
One Mole

- One mole of anything contains $6.022 \times 10^{23}$ entities.
  - 1 mol H = $6.022 \times 10^{23}$ atoms of H
  - 1 mol $H_2$ = $6.022 \times 10^{23}$ molecules of $H_2$
  - 1 mol $CH_4$ = $6.022 \times 10^{23}$ molecules of $CH_4$

One Mole of Elements

- Nickel(II) chloride
- Copper(II) sulfate
- Sodium chloride
- Cobalt(II) chloride
- Potassium dichromate

Moles to Number of Entities

$$\left(\frac{6.022 \times 10^{23} \text{ atoms}}{\text{mol}}\right) \text{ or } \left(\frac{\text{mol}}{6.022 \times 10^{23} \text{ atoms}}\right)$$

Example Calculations

- How many moles are present in $3.00 \times 10^{21}$ molecules of $C_2H_2$?

  $$3.00 \times 10^{21} \text{ molecules}$$
Moles to Mass

The Mole

- Calculate the mass of a single Mg atom, in grams, to 3 significant figures.

\[ ?g \text{ Mg} = 1 \text{ Mg atom} \]

- Calculate the number of atoms in one-millionth of a gram of Mg to 3 significant figures.

\[ ?\text{Mg atoms} = 1.00 \times 10^{-6} \text{ g Mg} \]

- How many atoms are contained in 1.67 moles of Mg?

\[ ?\text{Mg atoms} = 1.67 \text{ mol Mg} \]
The Mole

• How many moles of Mg atoms are present in 73.4 g of Mg?

? mol Mg = 73.4 g Mg

IT IS IMPERATIVE THAT YOU KNOW HOW TO DO THESE PROBLEMS!

Molar Mass

• The molar mass (MW) of any atom, molecule or compound is the mass (in grams) of one mole of that substance.
• The molar mass in grams is numerically equal to the atomic mass or molecular mass in amu.
  • 1 mole of hydrogen atoms = 1.01 g H
  • 1 mole of helium atoms = 4.00 g He
  • 1 mole of sodium atoms = 22.99 g Na

Formula Weights, Molecular Weights, and Moles

• To calculate the molar mass of a compound add atomic weights of each atom
• The molar mass of propane, C₃H₈, is:
  3 × C = 3 × 12.01 amu = 36.03 amu
  8 × H = 8 × 1.01 amu = 8.08 amu
  Molar mass = 44.11 amu
• The molar mass of calcium nitrate, Ca(NO₃)₂, is:
  1 × Ca = 1 × 40.08 amu = 40.08 amu
  2 × N = 2 × 14.01 amu = 28.02 amu
  6 × O = 6 × 16.00 amu = 96.00 amu
  Molar mass = 164.10 amu

Molecules to Moles

• What is the mass of 0.25 moles of CH₄?

\[ \text{g CH}_4 = 0.25 \text{ mol} \]
• Calculate the number of \( \text{C}_3\text{H}_8 \) molecules in 74.6 g of propane.

\[ ? \text{ molecules} = 74.6 \text{ g} \]

• What is the mass of 10.0 billion propane molecules?

\[ ? \text{ g} = 1.00 \times 10^{10} \text{ molecules} \]

• How many (a) moles, (b) molecules, and (c) oxygen atoms are contained in 60.0 g of ozone, \( \text{O}_3 \)? The layer of ozone in the stratosphere is very beneficial to life on earth.

\[ ? \text{ moles } \text{O}_3 = 60.0 \text{ g } \text{O}_3 \]

• Calculate the number of O atoms in 26.5 g of \( \text{Li}_2\text{CO}_3 \).

\[ ? \text{ O atoms} = 26.5 \text{ g } \text{Li}_2\text{CO}_3 \]
Formula Weights, Molecular Weights, and Moles

• Occasionally, we will use millimoles.
  • Symbol - mmol
  • 1000 mmol = 1 mol
• For example: oxalic acid (COOH)₂
  • 1 mol = 90.04 g
  • 1 mmol = 0.09004 g or 90.04 mg

Calculate the number of mmol in 0.234 g of oxalic acid, (COOH)₂.

7 mmol H₂C₂O₄ = 0.234 g H₂C₂O₄

An alternate method:

Problem Map

Percent Composition and Formulas of Compounds

• Determine the percent composition of C in C₃H₈.

\[
\text{mass %} = \frac{\text{no. atoms (atomic weight)}}{\text{molecular weight}} \times 100
\]

\[
\% \text{ C} = \frac{\text{mass C}}{\text{mass C}_3\text{H}_8} \times 100\%
\]
\[
= \frac{3 \times 12.01 \text{ g}}{44.11 \text{ g}} \times 100\%
\]
\[
= 81.68\%
\]
Derivation of Formulas from Elemental Composition

- **Empirical Formula** - smallest whole-number ratio of atoms present in a compound
- CH₂ is the empirical formula for alkenes
- No alkene exists that does not have a 1 C to 2 H's ratio
- **Molecular Formula** - actual numbers of atoms of each element present in a molecule of the compound
- Ethene – C₂H₄
- Pentene – C₅H₁₀

We determine the empirical and molecular formulas of a compound from the percent composition of the compound.

- percent composition is determined experimentally

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A compound contains 24.74% K, 34.76% Mn, and 40.50% O by mass. What is its empirical formula?

Make the simplifying assumption that we have 100.0 g of compound.

In 100.0 g of compound there are:
- 24.74 g of K
- 34.76 g of Mn
- 40.50 g of O

---

A sample of a compound contains 6.541 g of Co and 2.368 g of O. What is empirical formula for this compound?

?molCo = 6.541 g Co

?molO = 2.368 g O x

---

find smallest whole number ratio
Derivation of Formulas from Elemental Composition

• A sample of a compound contains 6.541 g of Co and 2.368 g of O. What is the empirical formula for this compound?

\[
\begin{align*}
\text{for Co} & : \frac{0.1110}{0.1110} = 1 \text{ Co} \\
\text{for O} & : \frac{0.1480}{0.1110} = 1.333 \text{ O}
\end{align*}
\]

multiply both by 3 to turn fraction to whole number

\[
\begin{align*}
1 \text{ Co} \times 3 & = 3 \text{ Co} \\
1.333 \text{ O} \times 3 & = 4 \text{ O}
\end{align*}
\]

Thus the compound’s formula is: \(\text{Co}_3\text{O}_4\).

Combustion Analysis

Empirical formulas are routinely determined by combustion analysis.

• A sample containing C, H, and O is combusted in excess oxygen to produce \(\text{CO}_2\) and \(\text{H}_2\text{O}\).

• The amount of \(\text{CO}_2\) gives the amount of C originally present in the sample.

• The amount of \(\text{H}_2\text{O}\) gives the amount of H originally present in the sample.

• Watch stoichiometry: 1 mol \(\text{H}_2\text{O}\) contains 2 mol H.

• The amount of O originally present in the sample is given by the difference in the amount of sample and the amount of C and H accounted for.

Combustion Analysis

• A compound contains only C, H, and O. A 0.1014 g-sample burns completely in oxygen to form 0.0609 g of water and 0.1486 g of \(\text{CO}_2\). Determine the simplest formula of the compound.

\[
\begin{align*}
0.1486 \text{ g CO}_2 \left(\frac{12.01 \text{ g C}}{44.01 \text{ g CO}_2}\right) & = 0.04055 \text{ g C} \\
0.0609 \text{ g H}_2\text{O} \left(\frac{2.016 \text{ g H}}{18.01 \text{ g H}_2\text{O}}\right) & = 0.00681 \text{ g H} \\
0.1014 \text{ g sample} - (0.04055 \text{ g C} + 0.00681 \text{ g H}) & = 0.0540
\end{align*}
\]
Combustion Analysis

C : \( \frac{0.003376}{0.003376} = 1 \)  
H : \( \frac{0.00674}{0.003376} = 2 \)  
O : \( \frac{0.003376}{0.003376} = 1 \)  

\( \text{CH}_2\text{O} \)

Molecular Formula Calculation

- If the molecular mass of the compound is 180 g/mol, what is the molecular formula?  

\( \text{CH}_2\text{O} \)  

\[ \text{FW} = 30.0 \text{ g/mol} \]  

\[ \begin{align*} 180 & = 6.0 \times 30.0 \\ &= 6.0 \end{align*} \]

Purity of Samples

- The percent purity of a sample of a substance is always represented as

\[ \text{% purity} = \frac{\text{mass of pure substance}}{\text{mass of sample}} \times 100\% \]

mass of sample includes impurities

Purity of Samples

- A bottle of sodium phosphate, \( \text{Na}_3\text{PO}_4 \), is 98.3% pure \( \text{Na}_3\text{PO}_4 \). What are the masses of \( \text{Na}_3\text{PO}_4 \) and impurities in 250 g of this sample of \( \text{Na}_3\text{PO}_4 \)?

\[ \begin{align*} \text{unit factor} &= \frac{98.3 \text{ g Na}_3\text{PO}_4}{100.0 \text{ g sample}} \\ \text{? g Na}_3\text{PO}_4 &= 250 \text{ g sample} \times \frac{98.3 \text{ g Na}_3\text{PO}_4}{100.0 \text{ g sample}} \\ &= 246 \text{ g Na}_3\text{PO}_4 \\ \text{? g impurities} &= 250 \text{ g sample} - 246 \text{ g Na}_3\text{PO}_4 \\ &= 4 \text{ g impurities} \end{align*} \]