CHAPTER 2

Chemical Formulas & Composition Stoichiometry
Atoms and Molecules

- Dalton’s Atomic Theory - 1808

John Dalton (1766-1844)
Atoms and Molecules

Atom

- the smallest particle of an element that maintains its identity through all chemical and physical changes
- consists of three fundamental particles
  - electron ($e^-$)
  - proton ($p^+$)
  - neutron ($n$)
- atomic number ($Z$) = # protons in the nucleus
- # protons = # electrons (electroneutrality!)
Atoms and Molecules

- **Molecule**
  - the smallest particle of a substance carrying its physical and chemical properties
  - usually consists of 2 or more atoms

- oxygen
- carbon monoxide
- hydrogen cyanide
- benzaldehyde
Chemical Formulas

- Chemical formula shows the chemical composition of the substance:
  - number of the atoms of each element present in the molecule or compound

- Substances differ from each other because their molecules are different
For the group of inert gases the atom and the molecule are equivalent:

- we say that these substances contain monoatomic molecules
Diatomic Molecules

- These elements exist as diatomic molecules
Triatomic Molecules

- If a substance is not an element but a compound, its molecule contains two or more kinds of atoms:

\[ \text{H}_2\text{O} \quad \text{CO}_2 \]

(water) (carbon dioxide)
Polyatomic Molecules

CH₄ (methane)

C₂H₅OH (ethyl alcohol)
Polyatomic Molecules

caffeine

sucrose
Atkins' Molecules

- One of the best books about molecules
- Written for general audience, not solely for chemists
Allotropes

- Different forms of the same element

Dioxygen

An $O_2$ molecule.

Ozone

An $O_3$ molecule.

117°
Ions

- Atoms are built of a nucleus and electrons orbiting around the nucleus.
- An atom may lose or gain one or more electrons - the resulting particle is called an ION.
  - If the atom loses electron(s), it becomes a cation (positively charged).
  - If the atom gains electron(s), it becomes an anion (positively charged).
Cations and Anions

- Positive ions - cations
  - one or more electrons less than neutral
  - \(\text{Na}^+, \text{Ca}^{2+}, \text{Al}^{3+}\)
  - \(\text{NH}_4^+\) - polyatomic cation

- Negative ions - anions
  - one or more electrons more than neutral
  - \(\text{F}^-, \text{O}^{2-}, \text{N}^{3-}\)
  - \(\text{SO}_4^{2-}, \text{PO}_4^{3-}\) - polyatomic anions

- Cations and anions can combine to form electroneutral ionic compounds
Ions and Ionic Compounds

- Sodium chloride
  - table salt is an ionic compound
The name of the cation should be followed by the name of the anion:

- NaCl
- KOH
- CaSO₄
- Al(OH)₃
- Mg(CH₃COO)₂
The total charge on the cations must equal the total charge on the anions which means that the compound must be neutral.

- ammonium bromide
- sodium oxide
- aluminum sulfate
- iron (II) nitrate
- copper(I) phosphate
Atomic Weights

- We know that an atom consists of electrons, protons, and neutrons.
- We know the masses of all three particles:
  \[
  m_p = 1.6726 \cdot 10^{-27} \text{ kg}
  \]
  \[
  m_n = 1.6749 \cdot 10^{-27} \text{ kg}
  \]
  \[
  m_e = 9.1094 \cdot 10^{-31} \text{ kg}
  \]
  \[
  \frac{m_p}{m_e} \approx 1840
  \]
- We can find the mass of the atom - the atomic weight.
Atomic Weights

- Unit of measure: a.m.u. = atomic mass unit
  - $m_p \approx m_n \approx 1$ a.m.u.
  - $m_e \approx 0$ a.m.u.

- Why do atomic weights of some elements deviate from integer so much?

- Answer: most elements consist of isotopes

Cl

17

35.4527
Isotopes

- Different atoms of the same element containing the same number of protons and electrons but different number of neutrons

- Atomic mass unit
  exactly $\frac{1}{12}$ of the mass of the carbon-12 atom
Molecular Weights

The sum of the atomic weights of all the atoms constituting the molecule

$M.W.(O_2) =$

$M.W.(C_2H_6O) =$
The Mole

- 1 atom or 1 molecule is a very small entity not convenient to operate with
- The masses we usually encounter in chemical experiments vary from milligrams to kilograms
  - Just like one dozen = 12 things
  - One mole = $6.022 \times 10^{23}$ things
- Avogadro’s number:
  \[ N_A = 6.022 \times 10^{23} \]
The Mole

$N_A = 6.022 \times 10^{23}$

- Why $6.022 \times 10^{23}$?
- This is the number of carbon atoms found in 12 g of the carbon-12 isotope.
- Molar mass - mass of one mole of atoms, molecules, ions, etc.
- Numerically equal to the atomic or molecular weight of the substance in grams:
  - $m (1 \text{ mole } H_2) = M_r(\text{H}_2) =$
  - $m (1 \text{ mole } \text{Fe}) = M_r(\text{Fe}) =$
The Mole: Example 1

Example: Calculate the mass of a single Mg atom in grams to 3 significant figures.
The Mole: Example 2

Example: How many $C_6H_{14}$ molecules are contained in 55 ml of hexane ($d = 0.78 \text{ g/ml}$).
Example: Calculate the number of O atoms in 26.5 g of lithium carbonate, Li$_2$CO$_3$. 
Percent Composition and Formulas of Compounds

- If the formula of a compound is known, its chemical composition can be expressed as the mass percent of each element in the compound (percent composition), and vice versa.

- When solving this kind of problems, we can use masses expressed in a.m.u. or in g/mol.
Percent Composition: Example 1

- What is the percent composition of each element in sodium chloride, NaCl?
Percent Composition: Example 2

- Calculate the percent composition of iron(III) sulfate, Fe$_2$(SO$_4$)$_3$, to 3 significant figures
Simplest (Empirical) Formula

- The *smallest* whole-number ratio of atoms present in the compound
- Molecular formula, on the other hand, indicates the *actual* number of atoms present in a molecule of the compound

\[
\begin{align*}
\text{H}_2\text{O} & \quad \text{H}_2\text{O}_2 \\
\text{water} & \quad \text{hydrogen peroxide}
\end{align*}
\]
The first high-temperature superconductor, prepared by Bednorz and Müller in 1986, contained 68.54% lanthanum, 15.68% copper, and 15.79% oxygen by mass. What was the simplest formula of this compound?
Empirical Formula: Example 2

A sample of a compound contains 6.541g of Co and 2.368g of O. What is its empirical formula?
Elemental Composition

- A combustion train for carbon-hydrogen analysis
- Percent composition is determined experimentally

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0.1195 g of a pure hydrocarbon was burned in a C-H combustion train to produce 0.3509 g of CO$_2$ and 0.1915 g of H$_2$O. Determine the masses of C and H in the sample, the percentage of these elements in this hydrocarbon, and the empirical formula of the compound.
0.1014 g sample of purified glucose was burned in a C-H combustion train to produce 0.1486 g of \( CO_2 \) and 0.0609 g of \( H_2O \). An elemental analysis showed that glucose contains only carbon, hydrogen, and oxygen. Determine the empirical formula of the compound.
Molecular Formula

- Indicates the **actual** number of atoms present in a molecule of the compound

- To determine the molecular formula for a molecular compound, **both its empirical formula and its molecular weight** must be known

- The molecular formula for a compound is either the same as, or an **integer** of, the empirical formula
A compound is found to contain 85.63% C and 14.37% H by mass. In another experiment its molar mass is found to be 56.1 g/mol. What is its molecular formula?
Other Examples

What mass of ammonium phosphate, \((\text{NH}_4)_3\text{PO}_4\), would contain 15.0 g of N?
Reading Assignment

- Read Chapter 2
- Learn Key Terms (p. 82)
- Go through Lecture 3 notes available on the class web site
- Read sections 3-1 through 3-5 of Chapter 3
Homework #1

Textbook problems (optional):
- Chapter 1 - 11, 13, 15, 18, 27, 29, 30, 32, 36, 41, 43, 47, 49, 57, 62, 68, 80
- Chapter 2 - 2, 3, 6, 13, 14, 17, 25, 29, 35, 38, 40, 46, 47, 49, 52, 55, 59, 62, 65, 68

OWL:
- Chapter 1 & 2 Exercises and Tutors - Optional
- Introductory math problems and Chapter 1 & 2 Homework problems - Required (due by 9/13)