Unit 3

Formulas and Equations

Objectives

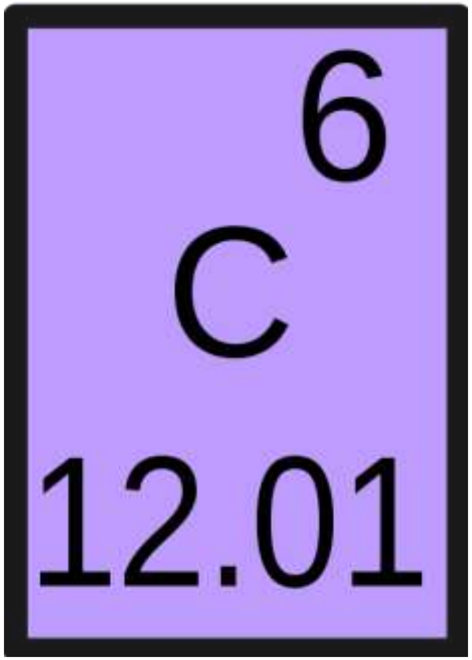
- Calculate atomic mass for an element.
- Explain the concept of the mole.
- Convert between mol and mass using the molar mass of a compound.
- Determine the number of molecules or atoms in a sample using Avogadro's Number.
- Calculate the percent composition of an element in a compound.
- Determine the empirical and molecular formula of a compound.
- Balance equations for simple chemical reactions
- Determine the limiting reactant.
- Calculate theoretical yield for a product.
- Determine the percent yield for a reaction.

Outline

I. Atomic Mass
   A. Calculating atomic mass
   B. Mass spectroscopy
II. Molar Mass
   A. Avogadro's number
   B. Converting between mol and atoms
   C. Molar Mass
   D. Converting between mol and grams
III. Compound Composition
   A. Percent composition
   B. Combustion analysis (experimental data)
   C. Finding the empirical formula
   D. Finding the molecular formula from the empirical formula
IV. Chemical Reactions
   A. Chemical equations
   B. Balancing chemical equations
V. Reaction Stoichiometry
   A. Amount of reactants and products
   B. Molar ratios
   C. Limiting reactants
   D. Calculating theoretical yield and percent yield

Atomic Mass

- Atomic mass is listed on the periodic table
- Mass of the element taking into account the relative abundance of all isotopes.
- Relative abundance = $\frac{\%}{100}$



$$\text{Atomic Mass} = \Sigma(RA_n A_n)$$

$$= RA_1(m_1) + RA_2(m_2) + RA_3(m_3) + \ldots$$

Atomic Mass

- ^{12}C is the standard for atomic mass
  - Assumed to have a mass of exactly 12 amu.
  - Masses of all other elements are given based on this mass.

Atomic Mass

- Calculate the average atomic mass of Mg given the following: ^{24}Mg is present 78.99% of the time, ^{25}Mg 10.00% and ^{26}Mg is present 11.01% of the time.

Data on isotope abundance is from the 1997 report of the IUPAC Subcommittee for Isotopic Abundance Measurements by K.J.R. Rosman, P.D.P. Taylor *Pure Appl. Chem.* ***1999, 71, 1593-1607.***
http://www.chem.ualberta.ca/~massspec/atomic_mass_abund.pdf

Atomic Mass

- Copper has two isotopes. ^{63}Cu is present 69.17% of the time. If the atomic mass of copper is 63.546 on the periodic table, calculate the mass number of the other isotope.

Data on isotope abundance is from the 1997 report of the IUPAC Subcommittee for Isotopic Abundance Measurements by K.J.R. Rosman, P.D.P. Taylor *Pure Appl. Chem.* ***1999, 71, 1593-1607.***
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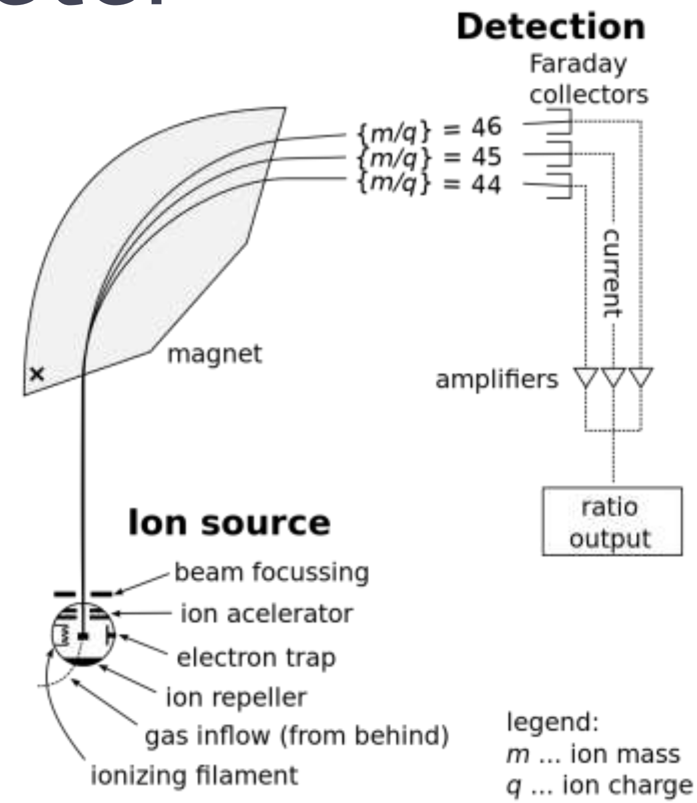
Mass Spectrophotmeter



ICPMS. EMSL. CC SA 2013. https://flic.kr/p/p7r9BT
Schematic of a mass spectrophotometer. US Geological Survey. PD 2008. http://pubs.usgs.gov/of/2001/ofr01-257/images/figure1.gif

Molar Mass

- ^{12}C is the standard for atomic mass
  - Assumed to have a mass of exactly 12 amu.
  - Masses of all other elements are given based on this mass.
- Chemistry deals in macroscopic
  - Mole = the number of atoms of ^{12}C in exactly 12 grams
  - Avogadro's Number = 6.022×10^{23} units
  - 12 g ^{12}C = 1 mol ^{12}C = 6.022×10^{23} atoms ^{12}C

Avogadro’s Number

- Named for Amedeo Avogadro
- Is unitless
- 1 mol = 6.022×10^{23} units
    - If the substance is an atom the units will be atoms
        - 1 mol Na = 6.022×10^{23} atoms
    - If the substance is a molecule; units = molecules
        - 1 mol O_2 = 6.022×10^{23} O_2 molecules
        - 1 mol NaCl = 6.022×10^{23} NaCl molecules

Avogadro's Number

- The mol is a huge number:
  - Mol Analogies
- Can be used to convert from mol to grams
  - Mol Concept Map

Application Quiz

- Calculate the number of atoms in a 5.24 mol sample of Na.

Application Quiz

- Calculate the number of Na atoms in a 4.21 mol sample of Na_2O.

Molar Mass

- Mass in grams of 1 mol of a substance.
  - Na = 22.99 g/mol
  - NaCl = 58.44 g/mol
  - H_2O = 18.02 g/mol
  - $(NH_4)_2SO_4$ = 132.17 g/mol

Application Quiz

- Calculate the mass of a single atom of Fe.

Application Quiz

- Calculate the number of atoms in 3.20 g of C.

Application Quiz

- Calculate the number of H atoms in 6.91 g of water.

Application Quiz

- You have 100.0 gram samples of potassium, sulfur and copper. Which sample has the greatest number of atoms?

Application Quiz

- You have 50.0 gram samples of water, dinitrogen monoxide and carbon dioxide. Which sample has the greatest number of oxygen atoms?

Mole Conversions

- Remember to always look at the information given in a question.
- Look for which units the question is looking for.
- Make a plan to convert where your units can cancel.
- Use the mole concept map to help until you are comfortable.

Percent Composition

$$\frac{\text{g element}}{\text{g total compound}} \times 100$$

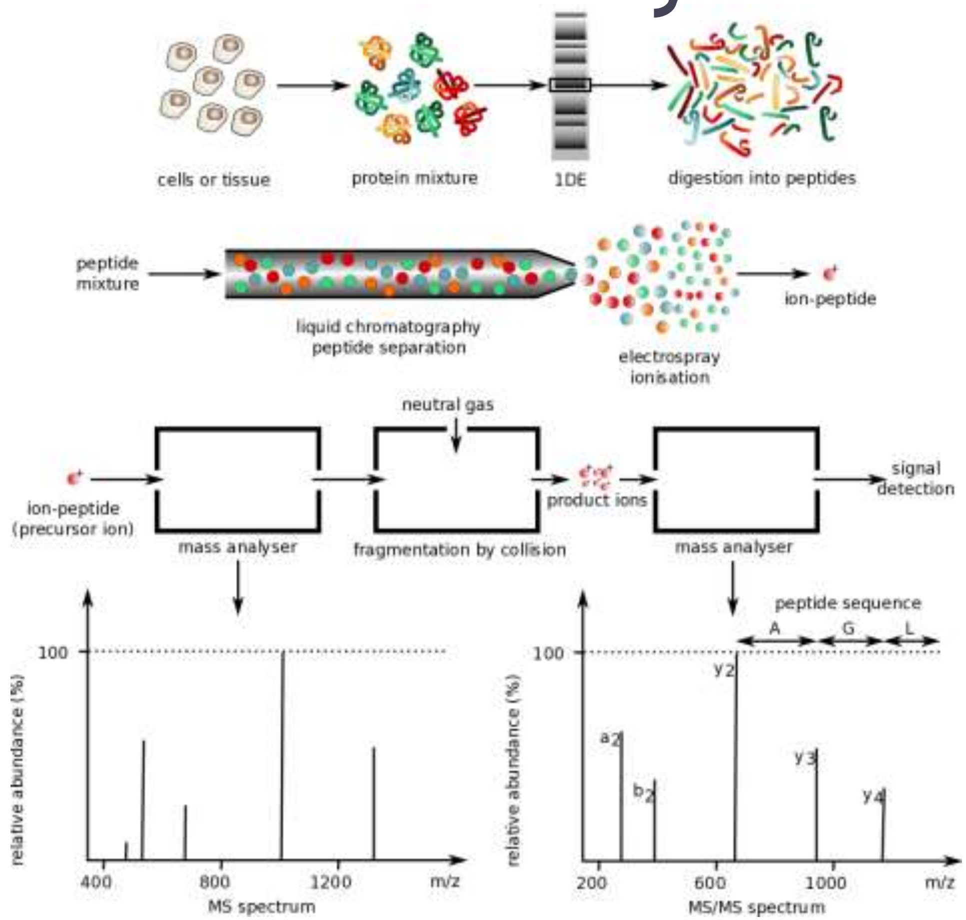
Application Quiz

- Calculate the percent composition of hydrogen in water.

Application Quiz

- Calculate the percent composition of hydrogen in sulfuric acid.

Combustion Analysis



Burned in the presence of O_2

C→ CO2, H → H_2O, etc

Mass Spectrometry Protocol. Emmanuel Barillot, Laurence Calzone, Philippe Hupé, Jean-Philippe Vert, Andrei Zinovyev, Computational Systems Biology of Cancer Chapman & Hall/CRC Mathematical & Computational Biology , 2012.
http://commons.wikimedia.org/wiki/File:Mass_spectrometry_protocol.png

Empirical Formulas

- Simplest ratio of elements.
- Molecular formula gives the actual number and types of atoms bonded together.

- Glucose
  - Molecular formula $C_6H_{12}O_6$
  - Empirical formula CH_2O
  - Here the empirical formula is different from the molecular by a multiple of $6(CH_2O)$

Empirical Formula Problems

1. If given units of percent assume a 100 g sample (%=g)
2. Convert g to mol using molar mass
3. You must have a whole number of mols. So divide by the smallest number of mols (mol -> #)
4. If still do not have only whole numbers of mols: Multiply all elements by the denominator. (mol -> #)
5. Use the whole number mol to write the empirical formula.
6. If you need to find Molecular formula Calculate the molar mass of empirical formula.
7. To find the ratio of Molecular / Empirical formula
   Divide Molecular formula Molar Mass by Empirical Formula Molar Mass.
8. Use the ratio to multiply all subscripts in the empirical formula to find the molecular formula.

Application Quiz

- A sample of an unknown compound is analyzed by a mass spectrophotometer. It is found to contain 64.80% C, 13.62 % H and 21.58 % O. The molar mass of the compound is 74.14 g/mol.
- Find the empirical and molecular formulas.

Application Quiz

- A sample of an unknown compound is analyzed by a mass spectrophotometer. It is found to contain 57.54% C, 3.45% H, and 39.01% F.
- Find the empirical and molecular formulas.

Application Quiz

- A sample of an unknown compound is analyzed by a mass spectrophotometer. It is found to contain 40.00% C, 6.68% H, and 53.33% O. The molar mass of the compound is 180 g/mol.
- Find the empirical and molecular formulas.

Chemical Reactions

- Represented with chemical equations

$$C_3H_8 + 5\,O_2 \rightarrow 3\,CO_2 + 4\,H_2O$$

- Reactants are placed on the left of the arrow.
- Products on placed on the right.
- Arrow = “reacts to produce”

Chemical Equations

- Matter cannot be created or destroyed in a chemical reaction.
- Chemical equations must be balanced.
- Same number of atoms of each type on left as on the right of the arrow.
- Coefficients indicate mol ratios.
- Subscripts indicate the state of matter.

Chemical Equations

$$C_3H_{8\,(l)} + 5\,O_{2\,(g)} \rightarrow 3\,CO_{2\,(g)} + 4\,H_2O_{\,(g)}$$

- Balanced 3 C, 8 H and 10 O atoms on each side.
- Equation is read as: 1 mol of propane reacts with 5 mol oxygen to produce 3 mol carbon dioxide and 4 mol water.

Balancing Chemical Equations

- Make a tally of all atoms in the reaction.
- Add coefficients to get the atoms to balance. (Cannot change subscripts.)
- Coefficients must be simplest (LCD) whole number ratios. (Occasionally depicted as fractions in literature—I will only use whole numbers on class activities).
- Balance H and O last.

Application Quiz

- Balance the following reaction:

$$MgCl_{2\,(aq)} + AgNO_{3\,(aq)} \rightarrow Mg(NO_3)_{2\,(aq)} + AgCl_{(s)}$$

Application Quiz

- Balance the following reaction:

$$H_2SO_{4\,(aq)} + NaOH_{(aq)} \rightarrow Na_2SO_{4\,(aq)} + H_2O_{(l)}$$

Application Quiz

- Balance the following reaction:

$$C_4H_{10\ (l)} + O_{2\ (g)} \rightarrow CO_{2\ (g)} + H_2O_{\ (g)}$$

Balanced Equations

- A balanced equation tells us:
  - The overall reaction.
  - The mol ratios of reactants and products.
  - The states of matter and form of compounds.
  - The number and types of atoms are conserved in a chemical reaction.

Balanced Equations

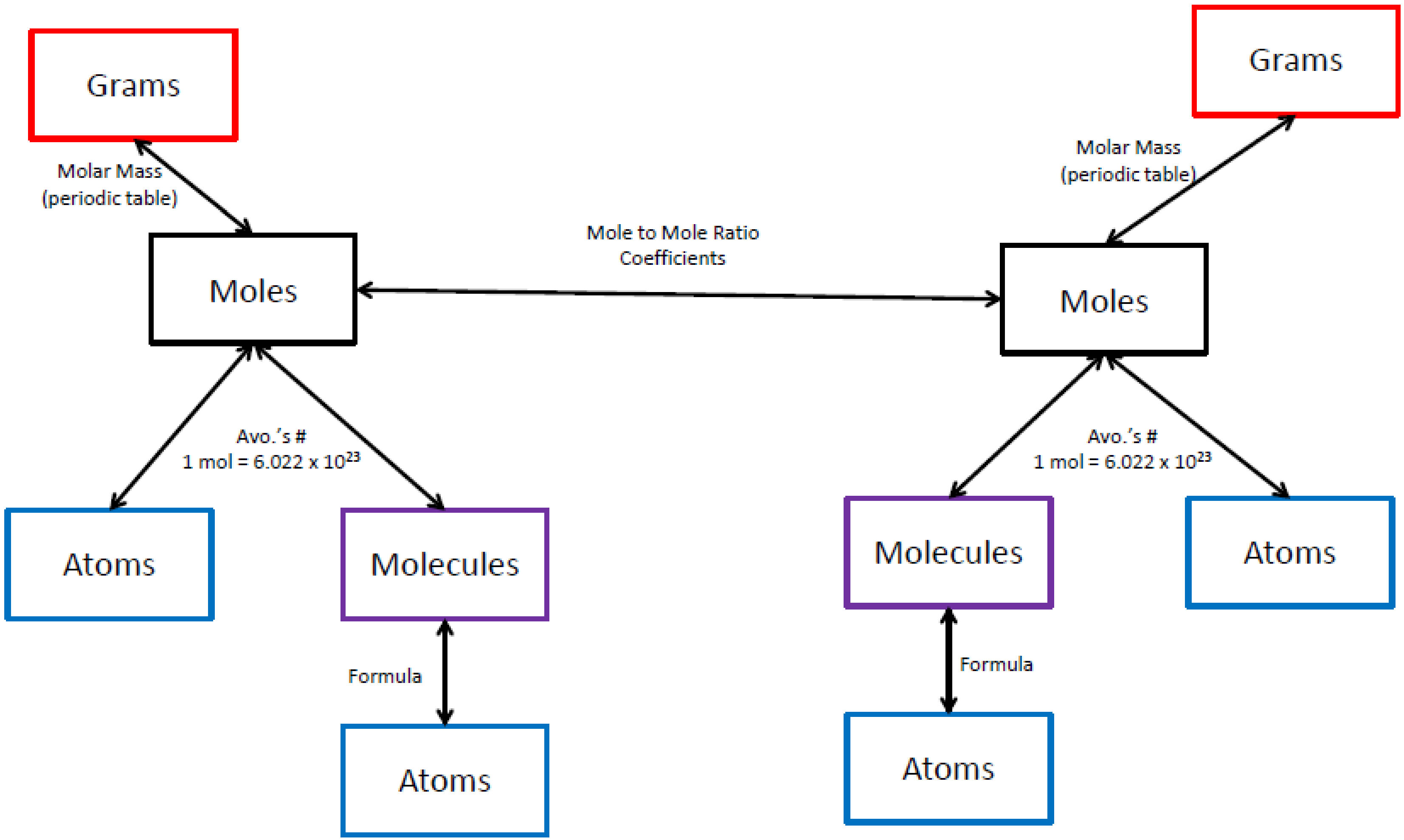
- A balanced equation does NOT tell us:
  - The mass of reactants or products involved in the reaction.
  - How the reaction occurred.

Reaction Stoichiometry

- Stoichiometry will allow us to calculate the mass of reactants and products involved in chemical reactions.

- The chemical equation MUST be balanced for this to work.

Mol Concept Map



Application Quiz

Consider the reaction below:

$$AgNO_{3\,(aq)} + Zn_{(s)} \rightarrow Zn(NO_3)_{2\,(aq)} + Ag_{(s)}$$

You begin with 14.1 g of $AgNO_3$.

- What mass of Zn is needed to react with $AgNO_3$?
- What mass of $Zn(NO_3)_2$ will be produced?
- How many Ag atoms are produced in the reaction?

Application Quiz

Consider the reaction below:

$Ca(NO_3)_{2\ (aq)} + K_3PO_{4\ (aq)} \rightarrow Ca_3(PO_4)_{2\ (s)} + KNO_{3\ (aq)}$

You begin with 22.18 g of K_3PO_4.

- What mass of $Ca(NO_3)_2$ is needed to react?
- What mass of $Ca_3(PO_4)_2$ will be produced?
- How many P atoms are involved in the reaction?

Limiting Reactant

- A chemical equation can only proceed while you have BOTH reactants left.
- Once one reactant is consumed the reaction CANNOT continue even if you have a lot of the other reactant left over.

Limiting Reactant

- The reactant that runs out is called the limiting reactant because it limits how much product can be formed.
- The reactant left over when the reaction is complete (limiting reactant has been used up) is called the excess reactant.

Limiting Reactant

- Consider sandwich makings:
  - You have –
    - An entire loaf of bread (12 pieces of bread)
    - 2 pieces of balogna

Limiting Reactant

12 pieces of bread (1 sandwich/ 2 pieces bread) = 6 sandwiches
2 pieces balogna (1 sandwich / 1 piece balogna) = 2 sandwiches

- You can only make 2 sandwiches.
- It does not matter that you have enough bread to make 6 sandwiches. Once the balogna is gone, the reaction (sandwich making) must stop.

Application Quiz

$$3Ca(NO_3)_{2\ (aq)} + 2K_3PO_{4\ (aq)} \rightarrow Ca_3(PO_4)_{2\ (s)} + 6KNO_{3\ (aq)}$$

You begin with 10.0 g of each reactant. Which is limiting?

Application Quiz

$$H_{2\ (g)} + Cl_{2\ (g)} \rightarrow HCl_{\ (aq)}$$

You begin with 7.15 g H_2 and 15.01 g Cl_2.
Which reactant is limiting?

Theoretical Yield

- The amount of product that can be made if all of the limiting reactant completely reacts.

Application Quiz

$$3Ca(NO_3)_{2\,(aq)} + 2K_3PO_{4\,(aq)} \rightarrow Ca_3(PO_4)_{2\,(s)} + 6KNO_{3\,(aq)}$$

What is the theoretical yield of calcium phosphate if 10.0 grams of each reactant are mixed together?

Application Quiz

$$H_{2\,(g)} + Cl_{2\,(g)} \rightarrow HCl_{\,(aq)}$$

You begin with 7.15 g H_2 and 15.01 g Cl_2.
What is the theoretical yield?

Percent Yield

- The amount of product actually made in the experiment divided by the theoretical yield and multiplied by 100.

$$\frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100$$

Application Quiz

$$H_{2\ (g)} + Cl_{2\ (g)} \rightarrow HCl_{\ (aq)}$$

In lab, you produced 12.81 grams of hydrochloric acid by the reaction above. What was the percent yield of the reaction if you should have produced 18.16 grams?