Chapter 3

Stoichiometry: Calculations with Chemical Formulas and Equations

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Chapter 3 suggested problems
10th Ed. and 11th Ed. - 3.x: 11, 13, 19, 21, 25, 33, 35, 37, 45, 47, 49, 57, 63, 69, 73, 75, 81, 86, 103

Class Notes

I. Chemical equations

A. Chemical equations - shorthand representations of chemical reactions

1. The reaction of aqueous silver (I) nitrate and aqueous ammonium chloride results in the formation of solid silver (I) chloride and aqueous ammonium nitrate

2. $AgNO_{3\ (aq)} + NH_4Cl_{(aq)} => AgCl_{(s)} + NH_4NO_{3\ (aq)}$

a. Reactants and products

b. Indications of state

c. Mass balance: coefficients vs. subscripts

i. $3\ Ba(NO_3)_{2\ (aq)} + 2\ Na_3PO_{4\ (aq)} => Ba_3(PO_4)_{2\ (s)} + 6\ NaNO_{3\ (aq)}$

ii. Note that subscripts are established by various factors such as ion charge and *never* (!) change during the process of mass balance. Only coefficients may be changed during mass balance.

II. Some simple patterns of chemical reactivity

A. By knowing a little about possible patterns of chemical behavior, we can correctly predict the outcome for thousands of reactions about which we really know very little

B. Double displacement reactions - "anion swapping reactions"

   1. $2\ KCl_{(aq)} + Pb(NO_3)_{2\ (aq)} \Rightarrow PbCl_{2\ (s)} + 2\ KNO_{3\ (aq)}$

C. Combustion reactions

   1. $C_5H_{12\ (l)} + 8\ O_{2\ (g)} \Rightarrow 5\ CO_{2\ (g)} + 6\ H_2O_{(g)}$

D. Combination and decomposition reactions

   1. Combination reactions: two or more smaller things combine to form one new larger thing

   2. Decomposition reactions: one larger thing breaks down into two or more smaller things

   3. Examples

      a. $2\ H_{2\ (g)} + O_{2\ (g)} \Rightarrow 2\ H_2O_{(g)}$

      b. $CaCO_{3\ (s)} \Rightarrow CaO_{(s)} + CO_{2\ (g)}$

E. Examples - don't worry about states (yet)

   1. $NaBr + Fe(NO_3)_3 \Rightarrow$

   2. $AlCl_3 + BaSO_4 \Rightarrow$

   3. The reaction of aqueous solutions of ammonium phosphate and calcium sulfite

   4. The reaction of aqueous solutions of sodium cyanide and gold (III) nitrate

   5. $CH_4 + O_2 \Rightarrow$

   6. The combustion of propanol

III. Avogadro's number and the mole

A. Avogadro's number

   1. The mass of a single C atom is 12.01 amu (from the atomic weight on the Periodic Table). How many C atoms are there in 12.01 g of C? (12.01 g C) x (1 kg / 1000 g) x (1 amu / 1.6605402 x 10^{-27} kg) x (1 C atom / 12.01 amu) = 6.022 x 10^{23} C atoms

   2. The mass of a single Au atom is 196.97 amu (from the atomic weight on the Periodic Table). How many Au atoms are there in 196.97 g of Au? (196.97 g Au) x (1 kg / 1000 g) x (1 amu / 1.6605402 x 10^{-27} kg) x (1 C atom / 196.97 amu) = 6.022 x 10^{23} Au atoms

3. The mass of a single glucose molecule is 180 amu (from the sum of the atomic weights of the elements from the Periodic Table). How many glucose molecules are there in 180 g of Au?
   (180 g glucose) x (1 kg / 1000 g) x (1 amu / 1.6605402 x 10^{-27} kg) x (1 glucose molecule / 180 amu) = 6.022 x 10^{23} glucose molecules

4. This holds true for any atom or molecule - the mass in grams of an atom or molecule equal to its weight in amu contains 6.022 x 10^{23} of that atom or molecule

   a. In other words, we have 1 mole of the substance when we have as many grams of a substance as its mass in amu

5. Avogadro's number = 6.022 x 10^{23}

6. 1 mole (x) = Avogadro's number of (x)

B. Note the relationship: the atomic weight on the Periodic Table is *both* the mass of a single atom in amu *and* the mass of a mole of the substance in grams

C. Molar mass - the sum of the weights of the moles of atoms in one mole of the compound (units of MW are g/mole) *note:* molar mass and molecular weight, while technically different, are used more ore less synonymously

1. H_2O

   a. The mass of a single molecule: 18.02 amu

   b. The mass of a mole of molecules: 18.02 g

2. CO_2

   a. The mass of a single molecule: 44.01 amu

   b. The mass of a mole of molecules: 44.01 g

3. $C_6H_{12}O_6$

   a. The mass of a single molecule: 180 amu

   b. The mass of a mole of molecules: 180 g

4. Diazinon is a pesticide with the molecular formula $C_{12}H_{21}N_2O_3PS$

   a. The mass of a single molecule: 304.34 amu

   b. The mass of a mole of molecules: 304.34 g

D. The linking relationship between the microscopic and the macroscopic is the mole. If we know how many moles of a substance we have, we also know how many atom/molecules of the substance we have. Conversely, if we know how many atom/molecules of the substance we have, we know how many moles of the substance we have.

1. How many moles of carbon are in one mole of diazinon? how many carbon atoms?
   12; (12) x (6.02 x 10^{23}) = 7.22 x 10^{24} carbon atoms

2. How many molecules are there in 1.4 moles of ethanol?
   (1.4 moles) x (6.02 x 10^{23} / 1 mole) = 8.43 x 10^{23} molecules

3. A sample contains 7.75 x 10^{15} molecules of ethanol, how many moles is this?
   (7.75 x 10^{15} molecules) x (1 mole / 6.02 x 10^{23}) = 1.29 x 10^{-8} mole

4. A sample of magnesium phosphate weighs 2.50 g, how many molecules is this?
   (2.50 g) x (1 mole / 262.87 g) x (6.02 x 10^{23} / 1 mole) = 5.73 x 10^{21} molecules

5. A chemical assay based on the detection of phosphorus can detect 5.65 pg of magnesium phosphate, how many P atoms are present?
   (5.65 pg) x (1 g / 10^{12} pg) x (1 mole / 262.87 g) x (6.02 x 10^{23} / 1 mole) = 1.29 x 10^{10} molecules x (2 P atoms / molecule) = 2.58 x 10^{10} P atoms

6. How many mg will 6.1 x 10^{20} butane molecules weigh?
   (6.1 x 10^{20} molecules) x (1 mole / 6.02 x 10^{23}) x (58.12 g / 1 mole) x (1000 mg / 1 g) = 58.9 mg butane

IV. Formula weights

A. Molecular weight - the weight of a single molecule of a compound in amu is equal to the sum of the masses of all of the atoms in the compound

1. H_2O - (2 x 1.008 amu) + (1 x 15.999 amu) = 18.02 amu

2. CO_2 - (1 x 12.01 amu) + (2 x 15.999 amu) = 44.01 amu

3. Glucose - $C_6H_{12}O_6$ - (6 x 12.01 amu) + (12 x 1.008 amu) + (6 x 15.999 amu) = 180.15 amu

4. $Al(OH)_3$ - (1 x 26.98 amu) + (3 x 16 amu) + (3 x 1.008 amu) = 78.0 amu

B. Formula weight - generally pertains to crystalline ionic solids, essentially the same as molecular weight (i.e., the weight of a single molecule) and calculated the same as molecular weight

C. Percent composition, or mass percentages

1. In a compound, the percent composition of an element is equal to [(the mass of the element divided by the mass of the compound) x 100]

2. Sulfur dioxide

   a. SO_2 - MW = 32.06 amu + (2 x 15.999 amu) = 64.06 amu

b. %S = (32.06 g / 64.06 g) * 100 = 50.05%

c. %O = (2 x 15.999 g / 64.06 g) * 100 = 49.95%

3. Glucose

a. $C_6H_{12}O_6$ - MW = 180 amu

b. %C = (6 x 12.01 g / 180.15 g) * 100 = 40.00%

c. %H = (12 * 1.008 g / 180.15 g) * 100 = 6.71%

d. %O = (6 * 15.999 g / 180.15 g) * 100 = 53.29%

D. Empirical formulas and elemental analysis (combustional analysis)

1. Empirical formula: the simplest whole number ratio of elements in a compound

a. Acetylene C_2H_2 and benzene C_6H_6: CH

b. Formaldehyde CH_2O and glucose $C_6H_{12}O_6$: CH_2O

c. For ionic compounds the empirical formula and the molecular formula are the same

2. For organic compounds, combustion of a known amount of a particular compound can reveal the number of moles of carbon, hydrogen, and oxygen in the compound

3. The combustion of 0.255 g of isopropyl alcohol produced 0.561 g of carbon dioxide and 0.306 g of water vapor.

a. grams C = (0.561 g CO_2) x (1 mol CO_2 / 44.0 g CO_2) x (1 mol C / 1 mol CO_2) x (1 mol C / 12.0 g C) = 0.153 g C

b. grams H = (0.306 g H_2O) x (1 mol H_2O/ 18.0 g H_2O) x (2 mol H / 1 mol H_2O) x (1 mol H / 1.01 g H) = 0.0343 g H

c. grams O = mass of sample - mass C - mass H = 0.255g - 0.153g - 0.0343g = 0.068g O

d. moles C = (0.153 g C) x (1 mol C / 12.0 g C) = 0.0128 mol C

e. moles H = (0.0343 g H) x (1 mol H / 1.01 g H) = 0.0340 mol H

f. moles O = (0.0343 g O) x (1 mol O / 16.0 g O) = 0.0043 mol O

g. Divide the number of moles of each by the smallest number of moles

i. moles C / moles O = 0.0128 mol / 0.0043 mol = 2.98

ii. moles H / moles O = 0.0340 mol / 0.0043 mol = 7.9

iii. moles O / moles O = 0.0043 mol / 0.0043 mol = 1

h. The empirical formula of isopropyl alcohol = $C_{2.98}H_{7.9}O_1$ = C_3H_8O

4. Combustion of a 0.225 g sample of caproic acid produced 0.512 g of carbon dioxide and 0.209 g of water vapor.

   a. grams C = (0.512 g CO_2) x (1 mol CO_2 / 44.0 g CO_2) x (1 mol C / 1 mol CO_2) x (1 mol C / 12.0 g C) = 0.140 g C

   b. grams H = (0.209 g H_2O) x (1 mol H_2O/ 18.0 g H_2O) x (2 mol H / 1 mol H_2O) x (1 mol H / 1.01 g H) = 0.0235 g H

   c. grams O = mass of sample - mass C - mass H = 0.225g - 0.140g - 0.0235 g = 0.0615g O

   d. moles C = (0.140 g C) x (1 mol C / 12.0 g C) = 0.0117 mol C

   e. moles H = (0.0235 g H) x (1 mol H / 1.01 g H) = 0.0233 mol H

   f. moles O = (0.0615 g O) x (1 mol O / 16.0 g O) = 0.00384 mol O

   g. Divide the number of moles of each by the smallest number of moles

      i. moles C / moles O = 0.0117 mol / 0.00384 mol = 3.05

      ii. moles H / moles O = 0.0233 mol / 0.00384 mol = 6.07

      iii. moles O / moles O = 0.00384 mol / 0.00384 mol = 1

   h. The empirical formula of caproic acid = $C_{3.05}H_{6.07}O_1$ = C_3H_6O

E. Determining molecular formulas from empirical formulas

1. If the empirical formula is known, determine the ratio of the molecular weight of the compound and the empirical formula weight

2. This ratio will be a whole number (or nearly so) by which the coefficients of the empirical formula are multiplied to give the molecular formula

3. The empirical formula of ascorbic acid is $C_3H_4O_3$. If the molecular weight of ascorbic acid is 176 amu, what is its molecular formula?

   a. The mass of the empirical formula is 88.0 amu

   b. 176 amu / 88.0 amu = 2

   c. 2 x ($C_3H_4O_3$) = $C_6H_8O_6$

4. Mesitylene has an empirical formula of C_3H_4. If its molecular weight is 121 amu, what is its correct molecular formula?

   a. The mass of the empirical formula is 40.0 amu

b. 121 amu / 40.0 amu = 3.02

c. 3 x (C_3H_4) = C_9H_{12}

V. Quantitative information from balanced equations

A. Definitions

1. According to BLB: "the area of study that examines the quantities of substances consumed and produced in chemical reactions"
2. My definition: calculation of the quantities of reactants and/or products based on their relationships in a balanced chemical equation
3. Note: a balanced chemical equation is essential to stoichiometry; a knowledge of molar masses is often also necessary

B. Mole relationships and conversion factors: in any balanced chemical equation equivalencies exist between all of the reactants and all of the products

1. $C_2H_5OH_{(l)} + 3\ O_{2\ (g)} \Rightarrow 2\ CO_{2\ (g)} + 3\ H_2O_{(g)}$

1 mol $C_2H_5OH(l)$ = 3 mol O_2 (g)	3 mol O_2 (g) = 2 mol CO_2 (g)	2 mol CO_2 (g) = 3 mol H_2O(g)
1 mol $C_2H_5OH(l)$ = 2 mol CO_2 (g)	3 mol O_2 (g) = 3 mol H_2O(g)	
1 mol $C_2H_5OH(l)$ = 3 mol H_2O(g)		

C. These equivalencies are useful when calculating amounts of reactants needed and/or amounts or product formed, both in terms of number of moles and mass

1. How many moles of ethanol (EtOH) must be burned to produce 16.7 moles of carbon dioxide?
(16.7 mol CO_2) x (1 mol EtOH / 2 mol CO_2) = 8.35 mol EtOH
2. The combustion of 2.78 moles of ethanol will produce how many moles of water vapor?
(2.78 mol EtOH) x (3 mol H_2O / 1 mol EtOH) = 8.34 mol H_2O
3. How many moles of oxygen are required for the complete combustion of 33.6 moles of ethanol?
(33.6 mol EtOH) x (3 mol O_2 / 1 mol EtOH) = 100.8 mol O_2
4. The combustion of ethanol produces 16.62 moles of carbon dioxide. How many moles of water vapor are also produced?
(16.62 mol CO_2) x (3 mol H_2O / 2 mol CO_2) = 24.93 mol H_2O
5. Mass conversions - these must *always* go through mole/mole conversions first; cannot do direct mass - mass conversions

a. How many grams of ethanol must be burned to produce 125 grams of carbon dioxide?
(125 g CO_2) x (1 mol CO_2 / 44.01 g CO_2) x (1 mol EtOH / 2 mol CO_2) x (46.07 g EtOH / 1 mol EtOH) = 65.4 g EtOH

b. How many grams of oxygen are required for the complete combustion of 1500 grams of ethanol?
(1500 g EtOH) x (1 mol EtOH / 46.07 g EtOH) x (3 mol O_2 / 1 mol EtOH) x (32.0 g O_2 / 1 mol O_2) = 3125.7 grams of oxygen

c. The combustion of a certain amount of ethanol produces 6.5 milligrams of carbon dioxide. How many milligrams of water vapor are also formed?
(6.5 mg CO_2) x (1 g CO_2 / 1000 mg CO_2) x (1 mol CO_2 / 44.01 g CO_2) x (3 mol H_2O / 2 mol CO_2) x (18.02 g H_2O / 1 mol H_2O) x (1000 mg H_2O / 1 g H_2O) = 3.99 mg H_2O

VI. Limiting reactants

A. Theoretical, actual, and percent yields and limiting reagents

1. The values calculated in stoichiometry problems are theoretical maximum values, i.e. they are the best values that can be obtained and only under ideal (if not perfect) conditions - these calculated values are called the *theoretical yields*

2. The real world is seldom ideal and never perfect - as a consequence there is almost always a disparity between the calculated theoretical yield and the actual amount obtained (*actual yield*) - this is always a measured value
theoretical: $C_2H_5OH_{(l)} + 3\ O_{2\ (g)} \Rightarrow 2\ CO_{2\ (g)} + 3\ H_2O_{(g)}$
actual (unbalanced): $C_2H_5OH_{(l)} + O_{2\ (g)} \Rightarrow C\ (s) + CO_{(g)} + CO_{2\ (g)} + 3\ H_2O_{(g)}$

3. Often the failure to obtain the theoretical yield is related to the presence of non-stoichiometric amounts of a reactant - the reactant of which there is stoichiometrically less is called the *limiting reagent* (or limiting reactant) - it is generally the reactant used up first - limits the amounts of product formed

4. The difference between the theoretical yield and the actual yield is expressed as the ratio of the two and called the percent yield - percent yield = (actual yield / theoretical yield) x 100

5. Examples

a. In an experiment 4.61 grams of ethanol are burned in the presence of 7.50 grams of oxygen. What mass of carbon dioxide is produced?
i. Which is the limiting reagent?
(4.61 g EtOH) x (1 mol EtOH / 46.07 g EtOH) x (2 mol CO_2 / 1 mol EtOH) x (44.01 g CO_2 / 1 mol CO_2) = 8.81 g CO_2
(7.50 g O_2) x (1 mol O_2 / 32.0 g O_2) x (2 mol CO_2 / 3 mol O_2) x (44.01 g CO_2 / 1 mol CO_2) = 6.88 g CO_2

ii. What is the theoretical yield? 6.88 g CO_2

iii. If only 3.56 grams of carbon dioxide are produced, what is

the percent yield?
(3.56 g / 6.88 g) x 100 = 51.7 %

b. While testing an experimental internal combustion engine 1.00 kg of ethanol is burned as fuel. The tests are conducted in a sealed chamber containing 2.50 kg of oxygen. What mass of carbon dioxide is produced?

    i. Which is the limiting reagent?
    (1.00 kg EtOH) x (1000 g EtOH / 1.00 kg EtOH) x (1 mol EtOH / 46.07 g EtOH) x (2 mol CO_2 / 1 mol EtOH) x (44.01 g CO_2 / 1 mol CO_2) = 1911 g CO_2
    (2.50 kg O_2) x (1000 g O_2 / 1 kg O_2) x (1 mol O_2 / 32.0 g O_2) x (2 mol CO_2 / 3 mol O_2) x (44.01 g CO_2 / 1 mol CO_2) = 2292 g CO_2

    ii. What is the theoretical yield? 1911 g CO_2

    iii. If 1875 grams of carbon dioxide are produced, what is the percent yield?
    (1875 g / 1911 g) x 100 = 98.1 %

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