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Principles of Chemistry, Tutorial 1

Definitions, Reactions and Stoichiometry

Materials are made up of smaller particles called atoms, which are bound together by different bonds to form compounds called molecules.

Every element in the periodic table has a chemical symbol chosen as the first letters of its Latin name. Generally elements are symbolized as following: ${}^{A}_{B}X$ where X is the elements symbol, A is the mass number and B is the atomic number.

Example: Carbon ${}^{12}_{6}C$

Atomic Number

The atomic number of an atom is equal to the number of protons in the atom, which is also equal to the number of electrons (in a neutral atom).

Mass Number

The mass number of an atom is equal to the sum of the number of protons and neutrons in the nucleus of the atom.

Isotopes

Isotopes are atoms with the same number of protons but with different number(s) of neutrons. For example two isotopes of chlorine are: ${}^{35}_{17}Cl$ and ${}^{37}_{17}Cl$

Ion

An ion is a charged atom. Two types of ions exist:

Cation – A positively charged atom (the neutral atom has lost one or more electrons)

Anion – A negatively changed atom (the neutral atom has gained on or more electrons)

Atomic Weight (AW)

The average mass of the different isotopes of an element based on their relative abundance:

$$AW = \sum_{i}^{N} Pi\mu i$$

Pi = relative abundance of isotope

μ_i = isotope mass

N = number of different isotopes (for a specific element)

Atomic Mass Unit (amu)

An atomic mass unit is a unit of measure for the weight of atoms. By definition 1 amu is 1/12 the weight of a carbon atom: ${}^{12}_{6}C$

Molecule

A molecule is a number of atoms bound together by chemical bonds.

$X_aY_bZ_c$

X, Y and Z represent the atoms in the molecule and a, b and c symbolize the number of X, Y and Z atoms respectively present in the molecule.

Example: the molecule glucose is represented as $C_6H_{12}O_6$

Molecular Weight (M_W)

The sum of the weights of each atom present in the molecule.

Avogadro's number (N_A)

Avogadro's number is defined as the number of ${}^{12}_{6}C$ atoms in 12 g of a ${}^{12}_{6}C$ sample.

Avogadro's number is a constant. $N_A = 6.022 \times 10^{23}$ atoms or molecules.

Avogadro's number is used to change units from number of atoms to weight.

Mole

A mole is the amount of material (atoms or molecules for example) which contains exactly Avogadro's number of particles.

Empirical Equation

The minimal ratio (in whole numbers) between the atoms present in a molecule.

Molecular Equation

A molecular equation represents the actual numbers of each atom present in a molecule.

Examples:

The molecular equation of benzene is C_6H_6 and the empirical equation is CH

In some cases the molecular and empirical equations are identical, for example CO_2

Chemical Reaction (Chemical Equation)

A chemical reaction is the reaction between two or more atoms to produce one or more products by the breaking of bonds and formation of new bonds.

Example: $Zn + S \rightarrow ZnS$

Reactants Products

A chemical equation must follow the law of conservation of mass and charge – the total number of atoms in the reactants and products must be equal and so too must be the overall charge. When dealing with chemical equations the first thing which MUST be done is to balance the equation:

Example:

$Ca + O_2 \rightarrow CaO$

This equation is unbalanced since there are more oxygen atoms in the reactants than in the products. The balanced equation is: $2Ca + O_2 \rightarrow 2CaO$

Balancing an equation:

Example:

$C_4H_{10} + O_2 \rightarrow CO_2 + H_2O$ (unbalanced equation)

(It is wise to first balance the atoms which appear in the least number of reactants or products)

Steps:

$C_4H_{10} + O_2 \rightarrow \mathbf{4}CO_2 + H_2O$ (to balance the carbon atoms)

$C_4H_{10} + O_2 \rightarrow 4CO_2 + \mathbf{5}H_2O$ (to balance the hydrogen atoms)

$C_4H_{10} + \mathbf{13/2}O_2 \rightarrow 4CO_2 + 5H_2O$ (to balance the oxygen atoms)

$\mathbf{2}C_4H_{10} + \mathbf{13}O_2 \rightarrow \mathbf{8}CO_2 + \mathbf{10}H_2O$ (everything is multiplied by two to give whole numbers)

Limiting Reagent

The reagent which is used up first and so determines the amounts of products produced.

Stoichiometry

The ratio between the elements and molecules used in a reaction.

Percentage Weight

The weight of a particular component, m_i , divided by the total weight, m_{TOT}, expressed as a percentage.

$$\frac{mi}{m_{TOT}} \times 100\%$$

Percentage volume

The volume of a particular component, V_i, divided by the total volume, V_{TOT}, expressed as a percentage.

$$\frac{Vi}{V_{TOT}} \times 100\%$$

^1H hydrogen-1 hydrogen 99.54%

^2H hydrogen-2 deuterium 0.0156%

^3H hydrogen-3 tritium negligible

H_2O water hydrogen monoxide

D_2O heavy water deuterium monoxide

Questions

1. Complete the following table:

Atom	Mass number A	Atomic number z	Charge	Number of protons	Number of neutrons	Number of electrons
$^{107}_{47}Ag$	107	47	0	47	60	47
Ag^{+1} (most abundant)	107	47	+1	47	60	46

2. An analysis of natural chlorine showed that 75.53% of the atoms are ^{35}Cl (A.W. = 34.968 amu) and 24.47% of the atoms are ^{37}Cl (A.W. = 36.956 amu). Calculate the atomic weight of natural chlorine.

3. A sulfuric acid solution (40% by weight) has a specific gravity of 1.31. What is the mass of sulfuric acid in 100 ml solution (40% by weight)? Assume that water at these conditions has a density of 1 g/cm^3.

$\rho_{solution} : \rho_{H_2O} = 1.31$ $\rho_{solution} = 1.31$

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2. $AW = \sum_{i=1}^{IV} p_i p_i = 75.53\% \times 34.968 + 0.2447 \times 36.956 = 35.4544\ 6216\ amu$

3. $m_{solution} = \rho_{sol.} \cdot V = 131\ g.$ $\% = \frac{m_{H_2SO_4}}{m_{solution}} = \frac{m_{H_2SO_4}}{131\ g} = 0.4$ $m_{H_2SO_4} = 52.4\ g$

4. Following is the reaction by which nitric acid is produced from NO_2

$3\ NO_{2(g)} + H_2O_{(l)} \rightarrow 2HNO_{3(l)} + NO_{(g)}$

a) Assume that 2 moles H_2O and 5 moles NO_2 are inserted into a container to react. Which of the reagents is the limiting reagent?

b) Calculate how much of the other reagent is left in excess.

5. An organic material, H_xC_ySz, is burnt according to the following reaction:

$a\ H_xC_ySz + b\ O_2 \rightarrow c\ SO_2 + d\ CO_2 + e\ H_2O$

At the end of the reaction 1.000 g of SO_2, 1.375 g of CO_2 and 0.8440 g H_2O are produced.

a) What is the empirical equation of the organic material?

b) Use the empirical equation to balance the chemical equation.

c) Assuming that the empirical formula is identical to the molecular formula, and that the initial mass of the organic material was 1.2098 g. What is the reaction yield?

6. A mixture of CuO and Cu_2O weighing 1.00 g is reduced using hydrogen to produce metallic copper and water according to the following equations:

Copper Oxide II: $CuO + H_2 \rightarrow Cu_{(s)} + H_2O$

Copper Oxide I: $Cu_2O + H_2 \rightarrow Cu_{(s)} + H_2O$

The total weight of the copper produced in the reactions is 0.839 g. Calculate the weight of CuO in the original mixture.

Fundamentals of Chemistry – Workshop 1

1. Density and specific gravity

A 5.0 ml bottle was filled with water at 25 °C. The weight of the water is 4.99 g. When petrol was put into an identical bottle at the same temperature, the mass of the petrol was found to be 3.58 g. What is the density and specific gravity of petrol?

2. How many hydrogen atoms make up 2.57 x 10^{-6} g hydrogen gas?

How many hydrogen molecules make up 2.57 x 10^{-6} g hydrogen gas?

Given: A.W. (H) = 1.01 g/mol

3. An analysis of caffeine showed that it is made up of the following atoms in the following percentage weights:

N = 28.58% H = 5.19% C = 49.48% O = 16.48%

a) Determine the empirical equation of caffeine

b) Given that the molecular weight of caffeine is 194 g/mol what is the molecular equation?

4. A mixture of chloride salt (MCl) and iodide salt (MI) weighs 2.083 g. It is known that there is a single charge on the metal, M^+. The salt mixture is dissolved in an aqueous solution and $AgNO_3$ is used to produce the precipitants AgCl and AgI. The weight of the dry precipitates is 3.781 g. The precipitate is reacted with chlorine gas according to the following reaction:

$$2AgI_{(s)} + Cl_{2(g)} \rightarrow 2AgCl_{(s)} + I_{2(g)}$$

At the end of this reaction, the total weight of pure AgCl is 2.866 g.

a) What is the percentage weight of the iodide anion in the original mixture?
b) Identify the cation M^+ by calculating its atomic weight.

5. Consider the following 0.1 M acidic solutions: phosphoric acid (H_3PO_4), HCl and H_2SO_4. Determine their concentrations in (a) mg/L; (b) eq/L (or N).

6. The following salts were dissolved in H_2O to produce a concentration of 115 mg/L as Na: Na_2SO_4, NaCl, Na_3PO_4. What is the concentration of the salts in each solution in mg/L?

1. $\rho = \frac{m}{V}$

$V_{H_2O} = V_{petrol}$

$\rho \propto m$

$\rho_{H_2O} = \frac{4.99g}{5mL} = 0.998\ g/mL$

$\rho_{petrol} = \frac{3.588g}{5mL} = 0.7176\ g/mL$

Specific gravity of petrol $= \frac{\rho_{petrol}}{\rho_{H_2O}} \approx 0.71743$

2. $M_{W_{H_2}} = 2.02\ g/mol$

$n_{H_2} = \frac{m}{M} = \frac{2.057\times10^{-6}g}{2.02g/mol} = 1.27227\times10^{-6}\ mol$

$\#H\ atom = 2 \cdot n_{H_2} \cdot N_A = 2\times1.27227\times10^{-6}\ mol \times 6.022\times10^{23}\ mol^{-1}$

$= 1.53232\times10^{18}$

$\#\ H_2\ molecules = \frac{\#H\ atom}{2} = 7.6616\times10^{17}$

3. Assume there's 100g caffeine.

a) there are 26.68g N. 5.19g H 49.48g C 16.45g O.

$n_{(N)} = 2.04142\ mol$ $n_{(H)} = 5.19\ mol$ $n_{(C)} = 4.123\ mol$ $n_{(O)} = 1.03\ mol$

$\div 1.03$

$n_{(N)} \approx 2$ $n_{(H)} \approx 5$ $n_{(C)} \approx 4$ $n_{(O)} \approx 1$.

The empirical equation: $C_4H_5ON_2$

b) The MW of empirical equation: $97g/mol \rightarrow \frac{1}{2}$ MW real.

Thus, the molecular formula: $C_8H_{10}O_2N_4$

4. $NaCl$ NaI

$x\ mol$ $y\ mol$

$NaCl + AgNO_3 \rightarrow AgCl + NaNO_3$

x x

$NaI + AgNO_3 \rightarrow AgI \downarrow + NaI$

y y

$x(M+35.5) + y(M+127) = 2.063$

$143.5x + 235y = 3.716$ ①

$2AgI + Cl_2 \rightarrow 2AgCl + I_2$

y y

$143.5(x+y) = 2.866$ ②

$x \approx 0.01$, $y = 0.01$

a) $\%\ weight_{(Cl)} = \frac{0.01mol\times127g/mol}{2.063g} \approx 61.96\%$

b) $0.01(M+35.5) + 0.01(M+127) = 2.063$

$0.01(2M + 162.5) = 2.063$

$2M + 162.5 = 206.3$

$M = \frac{206.3-162.5}{2} \approx 23$.

$M = Na$.

M^+ = Sodium Cation

5. Assume there's 1L solution

$m_{(H_3PO_4)} = n \cdot f = 9.8g$

$g/eq_{(H_3PO_4)} = \frac{98g/mol}{3} = \frac{98}{3}\ g/eq$

$eq/L_{(H_3PO_4)} = (9.8g \div \frac{98}{3} \cdot g^{-1}\ eq) \div 1L = 0.3\ eq/L$

Similarly

$g/eq_{(H_2CO_3)} = 0.1\ eq/L$

$g/eq_{(H_2SO_4)} = 0.2\ eq/L$

Eq(当量)：参与反应的有效成分质量；

1eq = 即与 1mol H^+/OH^- 或 1mol e^- 发生反应所需的物质质量(g)

(g/eq)克当量 = 物质的摩尔质量 ÷ 反应中等价单位数 n。（1eq 对应多少克物质 ⇒ 与 1mol H^+/OH^- 或 1mol e^- 反应需要多少物质）

1) 酸碱反应中 n = 可解离的 H^+/OH^- 数。

eg. HCl → H^+, n=1

(g/eq) = 36.5g/mol ÷ 1 = 36.5g/eq。

含义：36.5g HCl 可与 1 mol OH 发生反应，这即为反应为 eq。

eg. H_2SO_4 → $2H^+$ n=2。

(g/eq) = 98g/mol ÷ 2 = 49g/eq

49g H_2SO_4 的反应活性，等价于 36.5g HCl（都能中和 1mol OH）

2) 离子反应中(盐类) n = 离子电荷数(绝对值)。

eg. NaCl → Na^+, Cl^- → n=1

eg. $CaCl_2$ → Ca^{2+} Cl^- → n=2

含义：55.5g $CaCl_2$ 的离子活性如与其他离子结合能力，等价于 58.5g NaCl

3) 氧化还原反应：n = 转移电子数

eg. $Cr_2O_7^{2-}$ → $2Cr^{3+}$ 每个 Cr：+6 → +3，1 $K_2Cr_2O_7$ 含 2Cr

n = 2×3 = 6。

g/eq = 294g/mol ÷ 6 = 49 g/eq。

含义：49g $K_2Cr_2O_7$ 在反应中转移的电子个数，等价于转移 1mol 电子

eq/L = 当量浓度：eq/L = 溶质的克当量数 ÷ 溶液体积(L)

⇓

溶质质量 ÷ 溶质克当量

(溶质分能与 n mol H^+/OH^- 反应 或 转移 n mol e^-)

eg. 1L (aq). 58.5g NaCl.

g/eq (NaCl) = 58.5g/mol ÷ 1 = 58.5g/eq

eq/L = (m ÷ g/eq ÷ V) = (58.5g ÷ 58.5g/eq) ÷ 1L = 1eq

Tutorial Number 2

Atomic Spectra and the Bohr Model

Waves and Electromagnetic radiation – The dual nature of light and small particles

Classically, electromagnetic radiation can be described by wavelength, λ, or frequency, ν, where:

$$\nu = \frac{c}{\lambda}$$

λ: wavelength – the distance between two peaks [m]

ν: frequency – the number of cycles per unit time [Hz] or [s^{-1}]

c: speed of light (constant) $c = 3.0 \times 10^8$ m/s = 3.0×10^{10} cm/s

The energy of an electromagnetic wave:

$$E = h\nu = h\frac{c}{\lambda}$$

h: Plank's constant $h = 6.626 \times 10^{-34}$ J·s

Monochromatic light is light of only one wavelength (i.e. light of only one color).

The photoelectric effect

When electromagnetic radiation is projected onto a piece of metal, electrons are emitted from the surface. It turns out that the emission of electrons happens only when the radiation has a frequency greater than a certain minimum. The kinetic energy of the emitted electrons increases as the frequency of the radiation projected onto the surface increases.

$$E = E_0 + E_k$$

E_0 is the work function – the minimal amount of energy required to emit the electron

E_k is the kinetic energy of the emitted electron. $E_k = 1/2mv^2$

In quantum theory electromagnetic radiation is described as particles called photons.

Bohr's Model of the atom

Important! This model can be applied only for hydrogen atoms and hydrogen-like atoms such as He^{+} and Li^{+2} (atoms with only one electron).

The model is based on three assumptions:

1. The electron can move around the nucleus in a singular circular orbit with a fixed radius and an energy specific to the particular orbit. In other words, the energy of the electron is quantized.

   n is the principle quantum number and describes the energy level at which the electron is located. n may take the values n=1,2,3,… where n=1 is called the ground state and higher values of n, n=2,3,4,… are called excited states.

   r_n is the radius of the energy level n and is described by the following equation:

$$r_n = \frac{n^2}{z} a_0$$

   Where z is the number of protons in the nucleus of the atom and

$$a_0 = \frac{h^2}{4\pi k m e^2} = 0.05292 nm \cong 0.5\,\text{Å}$$

   h is planks constant, k is another constant, m is the mass of the electron and e is the charge of the electron.

   E_n is the energy of level n and is described by the following equation:

$$E_n = -R_H \frac{Z^2}{n^2}$$

   R_H is Rydberg's constant: $R_H = 2.18 \times 10^{-18}$ Joule = 2.18×10^{-11} erg =13.6 eV
   Z is the number of protons in the nucleus.

2. When an electron moves from orbit to orbit (or energy level to energy level) electromagnetic radiation is absorbed or emitted.

   Emission occurs when the final energy level is lower than the initial energy level

Absorption occurs when final energy level is higher than the initial energy level

The difference in energy between two levels is given by the Rydberg formula:

$$\Delta E = h\nu = E_f - E_i = R_H z^2 \left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right)$$

i = initial and f = final

The result of this energy quantization is that each element has characteristic emission spectra. Energy is NOT emitted in continuous spectra but rather as discrete values, which correlate to the specific energy differences between the different energy levels in the atom.

E_I, the ionization energy is the energy required to remove an electron from an atom indefinitely, turning the atoms into an ion.

$$E_I = R_H z^2 \left(\frac{1}{n_i^2} - \frac{1}{\infty^2}\right) = R_H z^2 \frac{1}{n_i^2} \qquad \Leftarrow n_f = \infty$$

3. The electron's orbital angular momentum in the n^{th} level is n times a constant, $\frac{h}{2\pi}$:

$$mVr = \frac{nh}{2\pi}$$

m is the mass of the electron

V is the angular velocity of the electron

R is the radius of the energy level n