Calculations Used in Analytical Chemistry

Some important units of measurement

SI Units

The International System of Units (SI) is based on 7 fundamental base units.

Base quantity		SI base unit	
Name of base quantity	**Symbol**	**Name of SI base unit**	**Symbol**
length	*l, x, r,* etc.	metre	m
mass	*m*	kilogram	kg
time, duration	*t*	second	s
electric current	*I, i*	ampere	A
thermodynamic temperature	*T*	kelvin	K
amount of substance	*n*	mole	mol
luminous intensity	I_v	candela	cd

The angstrom unit Å is a non-SI unit of length widely used to express the wavelength of very short radiation such as X-rays (1 Å = 0.1 nm).

Thus, typical X-radiation lies in the range of 0.1 to 10 Å.

Metric units of kilograms (kg), grams (g), milligrams (mg), or micrograms (µg) are used in the SI system.

Volumes of liquids are measured in units of liters (L), milliliters (mL), microliters (µL), and sometimes Nano liters (nL).

The liter, the SI unit of volume, is defined as exactly 10^{-3} m^3 . The milliliter is defined as 10^{-6} m^3 , or 1 cm^3 .

The Distinction Between Mass and Weight

Mass is an invariant measure of the quantity of matter in an object.

1. Weight is the force of attraction between an object and its surroundings, principally the earth. Because gravitational attraction varies with geographical location, the weight of an object depen

 2. Weight and mass are related by the familiar expression

$$w = mg$$

w is the weight of an object,

m is its mass, and g is the acceleration due to gravity.

The Mole

¬ The mole (abbreviated mol) is the SI unit for the amount of a chemical substance.

¬ It is always associated with specific microscopic entities such as atoms, molecules, ions, electrons, other particles, or specified groups of such particles as represented by a chemical formula.

¬ It is the amount of the specified substance that contains the same number of particles as the number of carbon atoms in exactly 12 grams of ^{12}C.

¬ This is Avogadro's number NA= 6.022 x 10^{23} .

¬ The molar mass M of a substance is the mass in grams of 1 mole of that substance.

The number of moles nX of a species X of molar mass MX is given by:

$$Amount\ X = nx =\ mX/\ MX$$

The molar mass of glucose is:

MX of $C_6H_{12}O_6$ = C(6x12) + H(12x1) + O(6x16) = **180** gm/mol

The Millimole

1 millimole = 1/1000 of a mole,

1 millimolar mass (mM) = 1/1000 of the molar mass.

1 mmol = 10^{-3} mol, and 10^3 mmol = 1 mol

Example:

Calculate the number of moles of aluminum present in (a) 108 g and (b) 13.5 g of the element. (Relative atomic mass: Al = 27).

Solution:

a–

$$\text{number of moles} = \frac{\text{mass}}{\text{molar mass}}$$

$$= \frac{108}{27} = 4 \text{ moles}$$

b–

$$\text{number of moles} = \frac{\text{mass}}{\text{molar mass}}$$

$$= \frac{13.5}{27} = 0.5 \text{ moles}$$

Example:

Calculate the number of moles of magnesium oxide, MgO in (a) 80 g and (b) 10 g of the compound. (Relative atomic mass: O = 16, Mg = 24)

Solution:

a) Mass of 1 mole of MgO

= (1 x 24) + (1 x 16)

= 40 g/mol

a–

$$\text{number of moles} = \frac{\text{mass}}{\text{molar mass}}$$

$$= \frac{80}{40} = 2 \text{ moles}$$

b–

$$\text{number of moles} = \frac{\text{mass}}{\text{molar mass}}$$

$$= \frac{10}{40} = 0.25 \text{ moles}$$

Example:

Calculate the mass of (a) 2 moles and (b) 0.25 moles of iron. (Relative atomic mass: Fe = 56)

Solution:

a) mass of 2 moles of iron
= number of moles × molar mass
= 2 × 56
= 112 g

b) mass of 0.25 mole of iron
= number of moles × molar mass
= 0.25 × 56
= 14 g

Calculation of moles by Avogadro number

Example: Calculate the number of moles of potassium in 1.25×10^{21} atoms K.

Answer

1mole   = 6.022×10^{23}

X   = 1.25×10^{21}

X= 1mole x 1.25×10^{21} / 6.022×10^{23}

X= 2.08×10^{-3} mol K

Example

What is the mass in grams of 2.01×10^{22} atoms of sulfur?

Example

How many O2 molecules are present in 0.470 g of oxygen gas?

Percent Composition of a Substance

Practice Exercise

Example 1

EDTA (ethylenediaminetetraacetic acid) is used as a food preservative and in the treatment of metallic lead poisoning. Calculate the percent composition of EDTA, $C_{10}H_{16}N_2O_8$

Answer

Molecular weight of EDTA= C(10x12)+ H(16x1)+ N(2x14)+O(8x16)

$$= 120+16+28+128= 292 \text{ gm/mol}$$

%C= (10x12/292)x100 = 41.09%

%H= (16x1/292)x100= 5.47%

%N= (2x14/292)x100= 9.58%

%O= (8x16/292)x100= 43.83%

41.09+5.47+9.58+43.83= 99.97

Example 2

If an analysis of sugar, CxHyOz, gave 40.0% C and 6.7% H, what is the percent oxygen?

Answer

%O= 100-(40.0+6.7)= 53.3%

Empirical Formula from Mass Composition

Example 1

In a laboratory experiment, 0.500 g of scandium was heated and allowed to react with oxygen from the air. The resulting product oxide had a mass of 0.767 g. Now, let's find the empirical formula for scandium oxide, Sc?O?.   mass number: Sc=44.96   O=16

Answer

The empirical formula is the simplest whole-number ratio of scandium and oxygen in the compound scandium oxide. This ratio is experimentally determined from the moles of each reactant. The moles of scandium are calculated as follows:

mol of Sc= 0.5/44.96=0.0111 mol Sc

weight of O= 0.767- 0.5= 0.267 g

mol of O= 0.267/16= 0.0166 mol O

Sc= 0.0111/0.0111=1

O= 0.0166/0.0111=1.5

$(Sc_1O_{1.5})$ X 2 = Sc_2O_3

Example 2

Iron can react with chlorine gas to give two different compounds, $FeCl_2$ and $FeCl_3$. If 0.558 g of metallic iron reacts with chlorine gas to yield 1.621 g of iron chloride, which iron compound is produced in the experiment? mass number: Fe=55.84   Cl=35.45

Answer

mol of Fe= 0.558/55.84= 0.01 mol Fe

weight of Cl= 1.621- 0.558= 1.063 g Cl

mol of Cl= 1.063/35.45= 0.03 mol Cl

Fe = 0.01/0.01=1

Cl= 0.03/ 0.01= 3

The compound is Fe Cl$_3$ (Ferric chloride)

Molecular Formula from Empirical Formula

Example 1

The empirical formula for fructose, or fruit sugar, is CH_2O. If the molar mass of fructose is 180 g/mol, find the actual molecular formula for the sugar.

Answer

We can indicate the molecular formula of fructose as $(CH_2O)n$. The molar mass of the empirical formula CH_2O is 12 g C + 2(1 g H) + 16 g O = 30 g/mol. Thus, the number of multiples of the empirical formula is:

n= 180/30= 6

Molecular formula of fructose is = 6 x (CH_2O)= $C_6H_{12}O_6$

Example 2

Ethylene dibromide was used as a grain pesticide until it was banned. Calculate (a) the empirical formula and (b) the molecular formula for ethylene dibromide given its approximate molar mass of 190 g/mol and its percent composition: 12.7% C, 2.1% H, and 85.1% Br.

mass number: Br=79.9

mol of C= 12.7/12= 1.05 mol C

mol of H= 2.1/ 1 = 2.1 mol H

mol of Br= 85.1/ 79.9= 1.06 mol Br

C= $1.05/1.05=1$

H= $2.1/1.05= 2$

Br= $1.06/1.05= 1$

a) empirical formula = $\mathbf{C_1H_2Br_1}$

The molar mass of the empirical formula CH_2Br = C(1x12)+H(2x1)+Br(1x79.9)= 93.9 g/mol

n= 190/ 93.9= **2**

b- molecular formula is $= n\ (CH_2Br)$

$$= 2(CH_2Br) = \mathbf{C_2H_4Br_2}$$

Solutions and their concentrations

In this subject, we describe the four fundamental ways of expressing solution concentration:

(1) molar concentration

(2) percent concentration

(3) normality concentration

(4) p-functions.

(1) Molar Concentration

The molar concentration cx of a solution of a solute species X is the number of moles of that species that is contained in 1 liter of the solution (not 1 L of the solvent).

$$c_x = \frac{n_X}{V}$$

$$\text{molar concentration} = \frac{\text{no. moles solute}}{\text{volume in liters}}$$

* The unit of molar concentration is molar, symbolized by M, which has the dimensions of mol/L, or mol L^{-1}.

** Molar concentration is also the number of millimoles of solute per

milliliter of solution.

$$1 \text{ M} = 1 \text{ mol L}^{-1} = 1 \frac{\text{mol}}{\text{L}} = 1 \text{ mmol L}^{-1} = 1 \frac{\text{mmol}}{\text{L}}$$

Example (1): Calculate the molar concentration of ethanol in an aqueous solution that contains 2.30 g of C_2H_5OH (46.07 g/mol) in 3.50 L of solution.

Solution:

To obtain the molar concentration, c_{C2H5OH}, we divide the amount by the volume. Thus:

$$c_{C_2H_5OH} = \frac{2.30 \text{ g } C_2H_5OH \times \dfrac{1 \text{ mol } C_2H_5OH}{46.07 \text{ g } C_2H_5OH}}{3.50 \text{ L}}$$

$$= 0.0143 \text{ mol } C_2H_5OH/L = 0.0143 \text{ M}$$

Example (2): Calculate the analytical molar concentrations of the solute species in an aqueous solution that contains 285 mg of trichloroacetic acid, Cl_3CCOOH (163.4 g/mol), in 10.0 mL.

Solution:

As in Example (1), we calculate the number of moles of Cl_3CCOOH, which we designate as HA, and divide by the volume of the solution, 10.0 mL, or 0.0100 L. Therefore:

$$\text{amount HA} = n_{HA} = 285 \text{ mg HA} \times \frac{1 \text{ g HA}}{1000 \text{ mg HA}} \times \frac{1 \text{ mol HA}}{163.4 \text{ g HA}}$$

$$= 1.744 \times 10^{-3} \text{ mol HA}$$

The molar analytical concentration, c_{HA}, is then:

$$c_{HA} = \frac{1.744 \times 10^{-3} \text{ mol HA}}{10.0 \text{ mL}} \times \frac{1000 \text{ mL}}{1 \text{ L}} = 0.174 \frac{\text{mol HA}}{\text{L}} = 0.174 \text{ M}$$

W in gm = **285/ 1000= 0.285 g**

M= (W/MW) x (1000/ V in ml)

M= (0.285/**163.4**) X **(1000/10)**

M= 0.00174 x 100 = 0.174 molar