CHAPTER 3

Calculations with Chemical Formulas and Equations

MOLECULAR WEIGHT (M. W.) Sum of the Atomic Weights of all atoms in a **MOLECULE** of a substance.	**FORMULA WEIGHT** (F. W.) Sum of the atomic Weights of all atoms in a **FORMULA UNIT** of a substance.
Can be used for: **MOLECULAR COMPOUNDS** only.	Can be used for both: - **IONIC COMPOUNDS** and - **MOLECULAR COMPOUNDS**
Example: MW (H_2O) = ? One H_2O molecule contains: 2 H atoms: 2 x 1.01 amu = 2.02 amu 1 O atom: 1 x 16.00 amu = 16.00 amu One **H_2O** molecule weighs → **18.02 amu**	Example: FW (Na_2CO_3) = ? One Formula Unit of Na_2CO_3 contains: 2 Na^+ ions: 2 x 22.99 amu = 45.98 amu 1 C atom: 1 x 12.01 amu = 12.01 amu 3 O atoms: 3 x 16.00 amu = 48.00 amu One **Na_2CO_3** formula unit weighs → **105.99 amu**

THE MOLE CONCEPT

- THE MOLE: - is the amount of substance that contains **6.02×10^{23}** **chemical units** such as:
  - atoms,
  - ions
  - molecules
  - formula units
  - electrons, etc.

6.023×10^{23} - is abbreviated **N_A**
- has been introduced in chemistry by the Italian scientist, Avogadro
- is referred to as **Avogadro's Number**

Examples:

1 mole H atoms ------------------------ contains: 6.023×10^{23} H atoms

1 mole H_2 molecules------------------- contains: 6.023×10^{23} H_2 molecules:

- $2 \times 6.023 \times 10^{23}$ H atoms = 1.20×10^{24} H atoms

1 mole H_2O molecules----------------- contains: 6.023×10^{23} H_2O molecules:

- $2 \times 6.023 \times 10^{23}$ H atoms = 12.05×10^{23} H atoms
- $1 \times 6.023 \times 10^{23}$ O atoms = 6.023×10^{23} O atoms

1 mole NaCl--------------------------- contains: 6.023×10^{23} formula units of NaCl:

- $1 \times 6.023 \times 10^{23}$ Na^+ ions
- $1 \times 6.023 \times 10^{23}$ Cl^- ions

1 mole Na_2CO_3----------------------- contains: 6.023×10^{23} formula units of Na_2CO_3:

- $2 \times 6.023 \times 10^{23}$ Na^+ ions = 12.05×10^{23} Na^+ ions
- $1 \times 6.023 \times 10^{23}$ CO_3^{2-} ions = 6.023×10^{23} CO_3^{2-} ions
- $1 \times 6.023 \times 10^{23}$ C atoms
- $3 \times 6.023 \times 10^{23}$ O atoms = 18.07×10^{23} O atoms

- MOLAR MASS (MM): - is the mass of one mole of substance
  - is equal to the Formula Weight expressed in grams

1 mole H_2O
- contains → 6.023×10^{23} molecules
- weighs → 18.02 g

1 mole Na_2CO_3
- contains → 6.02×10^{23} formula units
- weighs → 105.99 g

Examples:

1. Calculate the mass in grams of one He atom.

$$1\ \cancel{\text{He atom}} \times \frac{1\ \text{mol He atoms}}{6.02 \times 10^{23}\ \cancel{\text{He atoms}}} \times \frac{\qquad}{\qquad} = \qquad \text{g}$$

2. How many C atoms are there in 4.00×10^{-8} g of propane (C_3H_8)?

$$4.00 \times 10^{-8}\text{g } C_3H_8 \times \frac{\qquad}{\qquad} \times \frac{\qquad}{\qquad} \times \frac{\qquad}{\qquad}$$

NOTE: Set up units so that they cancel out

3. How many moles of Na atoms are there in 50.0 g of Na?

4. What is the mass of 6.30 moles of lead (II) sulfate ?

Formula of lead (**II**) sulfate: $\overset{\mathbf{2+}}{Pb}\overset{2-}{SO_4}$ → $PbSO_4$

$$? \text{ g } PbSO_4 = 6.30 \text{ moles } PbSO_4 \times \frac{\textbf{?????? g } \mathbf{PbSO_4}}{1 \text{ mole } PbSO_4}$$

1 mole $PbSO_4$ = Molar Mass of $PbSO_4$:

1 mole Pb	=	1 x 207.2 g	=	207.2 g
1 mole S	=	1 x 32.07 g	=	32.07 g
4 moles O	=	4 x 16.00 g	=	64.00 g
				303.3 g

$$? \text{ g } PbSO_4 = 6.30 \text{ moles } PbSO_4 \times \frac{303.3 \text{ g } PbSO_4}{1 \text{ mole } PbSO_4} = \mathbf{1.91 \times 10^3 \text{ g } PbSO_4}$$

5. Calculate the number of moles in 2.45 g of magnesium sulfate.

Formula of magnesium sulfate: $Mg^{2+}SO_4^{2-} \longrightarrow MgSO_4$

$$? \text{ moles } MgSO_4 = 2.45 \text{ g } MgSO_4 \times \frac{1 \text{ mole } MgSO_4}{?????\text{ g } MgSO_4}$$

1 mole $MgSO_4$ = Molar Mass of $MgSO_4$:

1 mole Mg	=	1 x 24.31 g	=	24.31 g
1 mole S	=	1 x 32.07 g	=	32.07 g
4 moles O	=	4 x 16.00 g	=	64.00 g
				120.38 g

$$? \text{ moles } MgSO_4 = 2.45 \text{ g } MgSO_4 \times \frac{1 \text{ mole } MgSO_4}{120.38 \text{ g } MgSO_4} = \mathbf{0.0204 \text{ moles } MgSO_4}$$

PERCENT COMPOSITION

- The percent composition of a compound is the mass percent of each element in the compound.

$$\text{Mass \% X} = \frac{\text{no. of X in formula x atomic mass of X}}{\text{molecular mass of compound}} \text{ x } 100$$

The recommended daily allowance of table salt (sodium chloride) is 2000. mg NaCl. How many mg of Na are contained in 2,000. mg NaCl?

First Step: Calculate the mass of 1 mole of compound

1 mole Na	=	1 x 22.9 g	=	22.99 g
1 mole Cl	=	1 x 35.45 g	=	35.45 g
		1 mole of NaCl	=	58.44 g

Second Step: Calculate the % by mass of each element in the compound

$$\% \text{ Na} = \frac{22.99 \text{ g}}{58.44 \text{ g}} \text{ x } 100 = 39.34\%$$

$$\% \text{ Cl} = \frac{35.45 \text{ g}}{58.44 \text{ g}} \text{ x } 100 = 60.66\%$$

Third Step: Check if the percentages add up to 100%

39.34 % Na + 60.66 % Cl = 100.00 %

How many mg of Na are contained in 2,000. mg NaCl ?

$$? \text{ mg Na} = 2{,}000. \text{ mg NaCl x } \frac{39.34 \text{ mg Na}}{100.00 \text{ mg NaCl}} = 786.8 \text{ mg Na}$$

Examples:

1. Calculate the percent composition of sodium phosphate (Na_3PO_4).

Calculate molar mass of sodium phosphate:

3 moles Na	=
1 mole P	=
4 moles O	=
1 mole Na_3PO_4	=

% Na = ———————— x 100 =

% P = ———————— x 100 =

% O = ———————— x 100 =

TOTAL % = 100.00 %

2. Calculate the mass percentage of copper in the natural ore malachite. The formula of malachite is $CuCO_3 \cdot Cu(OH)_2$

First: Calculate the mass of 1 mole of $CuCO_3 \cdot Cu(OH)_2$

2 moles Cu	=	2 x 63.55 g	=	127.1 g Cu
1 mole C	=	1 x12.01 g	=	12.01 g C
5 moles O	=	5 x 16.00 g	=	80.00 g O
2 moles H	=	2 x 1.01 g	=	2.02 g H
1 mole $CuCO_3 \cdot Cu(OH)_2$			=	221.1 g

$$\% \text{ Cu} = \frac{127.1 \text{ g}}{221.1 \text{ g}} \times 100 = 57.49\%$$

3. Calculate the mass of copper in 1.37 grams of copper (II) oxide (CuO)

1 mole Cu	=	1 x 63.55 g	=	63.55 g
1 mole O	=	1 x 16.00 g	=	16.00 g
		1 mole CuO	=	79.55 g

$$? \text{ g Cu} = \cancel{1.37 \text{ g CuO}} \times \frac{63.55 \text{ g Cu}}{\cancel{79.55 \text{ g CuO}}} = 1.09 \text{ g Cu}$$

4. Seawater contains 0.0065% (by mass) of bromine. How many grams of bromine are there in 2.50 L of seawater? The density of seawater is 1.025 g/cm^3.

CHEMICAL FORMULAS

- Formulas give information about the type, the number, and arrangement of atoms in a substance
- Two important type of formulas will be discussed and compared:

MOLECULAR FORMULAS	EMPIRICAL FORMULAS (Simplest Formulas)	
can be written for molecular compounds only	can be written for both molecular and ionic compounds	
- indicate the number of atoms of each kind in a molecule - are multiples of empirical formulas	indicate the smallest whole number ratio between the atoms or ions of a substance (smallest whole number subscripts)	Multiplier
H_2O_2 (hydrogen peroxide)	HO	2
H_2O	H_2O	1
C_2H_2 (acetylene)	CH	2
C_6H_6 (benzene)	CH	6
$C_6H_{12}O_6$ (glucose)	CH_2O	6
C_6H_{12} (cyclohexane)	CH_2	6
$C_6H_4Cl_2$	C_3H_2Cl	2
Does not exist for an Ionic Compound	NaCl	--
Does not exist for an ionic compound	SnO_2	--

Calculating the Empirical (Simplest Formula)

Information Required: - Percentage Composition by Mass, or
- Composition by weight

Example:

Tin (Sn) reacts with oxygen (O) to form an oxide of tin (Sn_aO_b), which contains 0.9913 g Sn and 0.2729 g O.

What is the Empirical Formula of the oxide ?

(that is: a = ? b = ?)

Step 1: MASS ⟶ MOLE

$$? \text{ moles Sn} = \text{0.9913 g Sn} \times \frac{\text{1 mole Sn}}{\text{118.71 g Sn}} = \text{0.008351 moles Sn atoms}$$

$$? \text{ moles O} = \text{0.2729 g O} \times \frac{\text{1 mole O}}{\text{16.00 g O}} = \text{0.01706 moles O atoms}$$

Step 2: DIVIDE BY SMALL

$$\text{Relative number of O atoms} = \frac{\text{0.01706 moles O}}{\text{0.008351 moles Sn}} = 2.043$$

$$\text{Relative number of Sn atoms} = \frac{\text{0.008351 moles Sn}}{\text{0.008351 moles Sn}} = 1.000$$

Empirical Formula: $Sn_{1.000}O_{2.043}$ ⟶ **SnO_2**

(includes experimental error)

Sample Problem # 1

Arsenic (As) reacts with oxygen (O) to form a compound that is 75.7 % As and 24.3 % O by mass.

What is the empirical formula of this oxide ?

Step 1: PERCENT → MASS

	75.7 % As	24.3% O
	↓	↓
Assume 100 g compound →	75.7 g As	24.3 g O

Step 2: MASS → MOLE

$$? \text{ moles As} = \cancel{75.7 \text{ g As}} \times \frac{1 \text{ mole As}}{\cancel{74.92 \text{ g As}}} = 1.01 \text{ moles As atoms}$$

$$? \text{ moles O} = \cancel{24.3 \text{ g O}} \times \frac{1 \text{ mole O}}{16.00 \text{ g O}} = 1.52 \text{ moles O atoms}$$

Step 3: DIVIDE BY SMALL

$$\text{Relative number of O atoms} = \frac{1.52 \text{ moles O}}{1.01 \text{ moles As}} = 1.50$$

$$\text{Relative number of As atoms} = \frac{1.01 \text{ moles As}}{1.01 \text{ moles As}} = 1.00$$

Empirical Formula: $As_{1.00}O_{1.50}$???????????

(subscipts must be whole numbers)

Step 4: MULTIPLY 'TIL WHOLE:

$(As_{1.00}O_{1.50})$ x 2 = As_2O_3

A Simple Rhyme for a Simple Formula
(to be remembered)

1. **Percent to Mass**
2. **Mass to Mole**
3. **Divide by small**
4. **Multiply 'til Whole**

Sample Problem # 1

A sample of Freon contains 0.423 g C, 2.50 g Cl, and 1.34 g F. What is the Empirical Formula of Freon?

1. Percent to Mass

This step may be skipped since masses are already given:

0.423 g C 2.50 g Cl 1.34 g F.

2. Mass to Mole

? moles C =

? moles Cl =

? moles F =

3. Divide by small

C =

Cl=

F=

Empirical Formula: ____________________

Finding the Molecular Formula

Information required: 1. Empirical Formula Ex: CH_2
2. Molecular Mass Ex: 56.0 amu

What is the Molecular Formula of this compound ?

Empirical Formula Mass of CH_2 is:

1 C = 1 x 12.0 amu = 12.0 amu +
2 H = 2 x 2.0 amu = 2.0 amu
14.0 amu

Molecular Formula: - cannot be ~~CH_2~~ → (14.0 amu ≠ 56.0 amu)
- multiplier is not 1

Consider the possible multipliers and the resulting Molecular Mass:

Multiplier (n):	1	2	3	4
Molecular Formula:	CH_2	C_2H_4	C_3H_6	C_4H_8
Molecular Mass(amu):	14.0	28.0	42.0	56.0

↑ correct Molecular Formula (yields correct Molecular Mass)

NOTE:

Molecular Mass = Multiplier x Empirical Formula Mass
MM = n x EFM
56.0 amu = 4 x 14.0 amu

It follows: $4 = \frac{56.0 \text{ amu}}{14.0 \text{ amu}}$

In General: $n = \frac{\text{Molecular Mass}}{\text{Empirical Formula Mass}}$

Sample Problem 1

The empirical formula for benzene is CH. The molecular mass of benzene is 78 amu. What is the molecular formula of benzene?

Empirical Formula Mass of CH is:

$$1\ C = 1 \times 12\ amu = 12\ amu\ +$$
$$1\ H = 1 \times 1\ amu = 1\ amu$$
$$13\ amu$$

Molecular Formula: $(CH)_n$ $n = ?$

$$n = \frac{\text{Molecular Mass}}{\text{Empirical Formula Mass}} = \frac{78\ amu}{13\ amu} = \mathbf{6}$$

Molecular Formula: $(CH)_6$ → $\mathbf{C_6H_6}$

Sample Problem 2:

A compound whose empirical formula is C_3H_2Cl has a Molecular Mass of 147.0 amu. What is the Molecular Formula ?

Empirical Formula Mass of C_3H_2Cl is:

$$3\ C = 3 \times 12.0\ amu = 36.0\ amu\ +$$
$$2\ H = 2 \times 1.0\ amu = 2.0\ amu$$
$$1\ Cl = 1 \times 35.5\ amu = 35.5\ amu$$
$$73.5\ amu$$

Molecular Formula: $(C_3H_2Cl)_n$ $n = ?$

$$n = \frac{\text{Molecular Mass}}{\text{Empirical Formula Mass}} = \frac{147\ amu}{73.5\ amu} = \mathbf{2}$$

Molecular Formula: $(C_3H_2Cl)_2$ → $\mathbf{C_6H_4Cl_2}$