

CHAPTER 3

## Calculations with Chemical Formulas and Equations

<p style="text-align: center;"><b>MOLECULAR WEIGHT</b> (M. W.)</p> <p>Sum of the Atomic Weights of all atoms in a <b>MOLECULE</b> of a substance.</p>	<p style="text-align: center;"><b>FORMULA WEIGHT</b> (F. W.)</p> <p>Sum of the atomic Weights of all atoms in a <b>FORMULA UNIT</b> of a substance.</p>
<p>Can be used for: <b>MOLECULAR COMPOUNDS</b> only.</p>	<p>Can be used for both: - <b>IONIC COMPOUNDS</b> and - <b>MOLECULAR COMPOUNDS</b></p>
<p>Example:</p> <p>MW (H<sub>2</sub>O) = ?</p> <p>One H<sub>2</sub>O molecule contains:</p> <p>2 H atoms: 2 x 1.01 amu = 2.02 amu</p> <p>1 O atom: 1 x 16.00 amu = 16.00 amu</p> <div style="text-align: center;"> </div> <p>One <b>H<sub>2</sub>O</b> molecule weighs <b>18.02 amu</b></p>	<p>Example:</p> <p>FW (Na<sub>2</sub>CO<sub>3</sub>) = ?</p> <p>One Formula Unit of Na<sub>2</sub>CO<sub>3</sub> contains:</p> <p>2 Na<sup>+</sup> ions: 2 x 22.99 amu = 45.98 amu</p> <p>1 C atom: 1 x 12.01 amu = 12.01 amu</p> <p>3 O atoms: 3 x 16.00 amu = 48.00 amu</p> <div style="text-align: center;"> </div> <p>One <b>Na<sub>2</sub>CO<sub>3</sub></b> formula unit weighs <b>105.99 amu</b></p>

<b>THE MOLE CONCEPT</b>
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- THE MOLE: - is the amount of substance that contains  $6.02 \times 10^{23}$  **chemical units** such as:
  - atoms,
  - ions
  - molecules
  - formula units
  - electrons, etc.

$6.023 \times 10^{23}$  - 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:  $6.023 \times 10^{23}$  H atoms

1 mole H<sub>2</sub> molecules----- contains:  $6.023 \times 10^{23}$  H<sub>2</sub> molecules:

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

1 mole H<sub>2</sub>O molecules----- contains:  $6.023 \times 10^{23}$  H<sub>2</sub>O molecules:

$$- 2 \times 6.023 \times 10^{23} \text{ H atoms} = 12.05 \times 10^{23} \text{ H atoms}$$

$$- 1 \times 6.023 \times 10^{23} \text{ O atoms} = 6.023 \times 10^{23} \text{ O atoms}$$

1 mole NaCl----- contains:  $6.023 \times 10^{23}$  formula units of NaCl:

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

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

1 mole Na<sub>2</sub>CO<sub>3</sub>----- contains:  $6.023 \times 10^{23}$  formula units of Na<sub>2</sub>CO<sub>3</sub>:

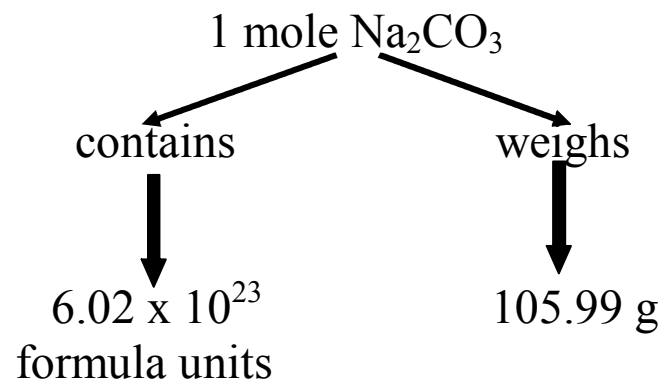
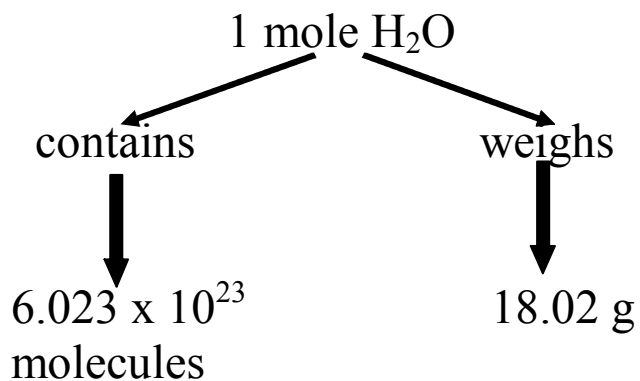
$$- 2 \times 6.023 \times 10^{23} \text{ Na}^+ \text{ ions} = 12.05 \times 10^{23} \text{ Na}^+ \text{ ions}$$

$$- 1 \times 6.023 \times 10^{23} \text{ CO}_3^{2-} \text{ ions} = 6.023 \times 10^{23} \text{ CO}_3^{2-} \text{ ions}$$

$$- 1 \times 6.023 \times 10^{23} \text{ C atoms}$$

$$- 3 \times 6.023 \times 10^{23} \text{ O atoms} = 18.07 \times 10^{23} \text{ O atoms}$$

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

**Examples:**

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

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

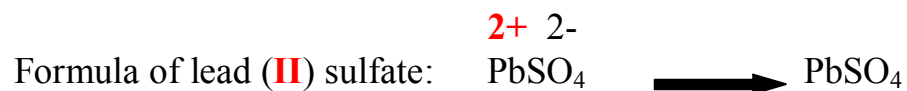
2. How many C atoms are there in  $4.00 \times 10^{-8}$  g of propane ( $\text{C}_3\text{H}_8$ )?

$$4.00 \times 10^{-8} \text{ g C}_3\text{H}_8 \times \text{_____} \times \text{_____} \times \text{_____}$$

**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 ?



$$? \text{ g PbSO}_4 = 6.30 \text{ moles PbSO}_4 \times \frac{\text{????? g PbSO}_4}{1 \text{ mole PbSO}_4}$$

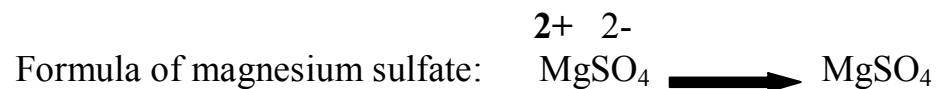
1 mole PbSO<sub>4</sub> = Molar Mass of PbSO<sub>4</sub> :

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.



$$? \text{ moles MgSO}_4 = 2.45 \text{ g MgSO}_4 \times \frac{1 \text{ mole MgSO}_4}{\text{????? g MgSO}_4}$$

1 mole MgSO<sub>4</sub> = Molar Mass of MgSO<sub>4</sub> :

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 =	<u>64.00 g</u>

**120.38 g**

$$? \text{ moles MgSO}_4 = 2.45 \text{ g MgSO}_4 \times \frac{1 \text{ mole MgSO}_4}{120.38 \text{ g MgSO}_4} = \text{0.0204 moles MgSO}_4$$

**PERCENT COMPOSITION**

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

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

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

$$\begin{array}{rclclcl} 1 \text{ mole Na} & = & 1 \times 22.9 \text{ g} & = & 22.99 \text{ g} \\ 1 \text{ mole Cl} & = & 1 \times 35.45 \text{ g} & = & \underline{35.45 \text{ g}} \\ & & 1 \text{ mole of NaCl} & = & 58.44 \text{ g} \end{array}$$

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

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

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

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

$$39.34 \% \text{ Na} + 60.66 \% \text{ Cl} = 100.00 \%$$

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

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

**Examples:**

1. Calculate the percent composition of sodium phosphate ( $\text{Na}_3\text{PO}_4$ ).

Calculate molar mass of sodium phosphate:

$$\begin{array}{rcl} 3 \text{ moles Na} & = & \\ 1 \text{ mole P} & = & \\ 4 \text{ moles O} & = & \end{array}$$

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$$1 \text{ mole Na}_3\text{PO}_4 =$$

$$\% \text{ Na} = \frac{\quad}{\quad} \times 100 =$$

$$\% \text{ P} = \frac{\quad}{\quad} \times 100 =$$

$$\% \text{ O} = \frac{\quad}{\quad} \times 100 =$$

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$$\text{TOTAL \%} = 100.00 \%$$

2. Calculate the mass percentage of copper in the natural ore malachite. The formula of malachite is  $\text{CuCO}_3 \cdot \text{Cu}(\text{OH})_2$

First: Calculate the mass of 1 mole of  $\text{CuCO}_3 \cdot \text{Cu}(\text{OH})_2$

$$\begin{array}{rclcl} 2 \text{ moles Cu} & = & 2 \times 63.55 \text{ g} & = & 127.1 \text{ g Cu} \\ 1 \text{ mole C} & = & 1 \times 12.01 \text{ g} & = & 12.01 \text{ g C} \\ 5 \text{ moles O} & = & 5 \times 16.00 \text{ g} & = & 80.00 \text{ g O} \\ 2 \text{ moles H} & = & 2 \times 1.01 \text{ g} & = & 2.02 \text{ g H} \end{array}$$

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$$1 \text{ mole CuCO}_3 \cdot \text{Cu}(\text{OH})_2 = 221.1 \text{ g}$$

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

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

$$\begin{array}{rclcl} 1 \text{ mole Cu} & = & 1 \times 63.55 \text{ g} & = & 63.55 \text{ g} \\ 1 \text{ mole O} & = & 1 \times 16.00 \text{ g} & = & 16.00 \text{ g} \end{array}$$

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$$1 \text{ mole CuO} \quad = \quad 79.55 \text{ g}$$

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

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<sup>3</sup>.



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:

<b>MOLECULAR FORMULAS</b>	<b>EMPIRICAL FORMULAS (Simplest Formulas)</b>	
can be written for <b>molecular compounds only</b>	can be written for <b>both molecular and ionic compounds</b>	
- indicate the <b>number of atoms of each kind in a molecule</b> - are multiples of empirical formulas	indicate the <b>smallest whole number ratio between the atoms or ions</b> of a substance (smallest whole number subscripts)	
		Multiplier
H <sub>2</sub> O <sub>2</sub> (hydrogen peroxide)	HO	2
H <sub>2</sub> O	H <sub>2</sub> O	1
C <sub>2</sub> H <sub>2</sub> (acetylene)	CH	2
C <sub>6</sub> H <sub>6</sub> (benzene)	CH	6
C <sub>6</sub> H <sub>12</sub> O <sub>6</sub> (glucose)	CH <sub>2</sub> O	6
C <sub>6</sub> H <sub>12</sub> (cyclohexane)	CH <sub>2</sub>	6
C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	C <sub>3</sub> H <sub>2</sub> Cl	2
Does not exist for an Ionic Compound	NaCl	--
Does not exist for an ionic compound	SnO <sub>2</sub>	--

### 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 ( $\text{Sn}_a\text{O}_b$ ), 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 $\longrightarrow$ MOLE

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

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

#### Step 2: DIVIDE BY SMALL

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

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

Empirical Formula:  $\text{Sn}_{1.000}\text{O}_{2.043} \longrightarrow \text{SnO}_2$   
(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<sub>1.00</sub>O<sub>1.50</sub> ??????????**  
 (subscripts must be whole numbers)

**Step 4: MULTIPLY 'TIL WHOLE:**

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: \_\_\_\_\_



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?

$$\begin{array}{l} \text{Empirical Formula Mass of CH is:} \\ 1 \text{ C} = 1 \times 12 \text{ amu} = 12 \text{ amu} + \\ 1 \text{ H} = 1 \times 1 \text{ amu} = 1 \text{ amu} \\ \hline 13 \text{ amu} \end{array}$$

$$\begin{array}{l} \text{Molecular Formula: } (\text{CH})_n \quad n = ? \\ \text{Molecular Mass} \quad 78 \text{ amu} \\ n = \frac{\text{Molecular Mass}}{\text{Empirical Formula Mass}} = \frac{78 \text{ amu}}{13 \text{ amu}} = 6 \end{array}$$

Sample Problem 2:

A compound whose empirical formula is  $\text{C}_3\text{H}_2\text{Cl}$  has a Molecular Mass of 147.0 amu. What is the Molecular Formula ?

$$\begin{array}{l} \text{Empirical Formula Mass of } \text{C}_3\text{H}_2\text{Cl} \text{ is:} \\ 3 \text{ C} = 3 \times 12.0 \text{ amu} = 36.0 \text{ amu} + \\ 2 \text{ H} = 2 \times 1.0 \text{ amu} = 2.0 \text{ amu} \\ 1 \text{ Cl} = 1 \times 35.5 \text{ amu} = 35.5 \text{ amu} \\ \hline 73.5 \text{ amu} \end{array}$$

$$\begin{array}{l} \text{Molecular Formula: } (\text{C}_3\text{H}_2\text{Cl})_n \quad n = ? \\ \text{Molecular Mass} \quad 147 \text{ amu} \\ n = \frac{\text{Molecular Mass}}{\text{Empirical Formula Mass}} = \frac{147 \text{ amu}}{73.5 \text{ amu}} = 2 \end{array}$$

