THE MOLE CONCEPT

- Chemists find it more convenient to use ***mass relationships*** in the laboratory, while ***chemical reactions*** depend on the ***number of atoms*** present.
- In order to relate the ***mass and number of atoms***, chemists use the SI unit ***mole*** (abbreviated ***mol***).
- The number of ***particles*** in a ***mole*** is called ***Avogadro's number*** and is ***6.02x10 ^{23}***.

1 mol of H atoms………contains: **6.02 x 10^{23}** H atoms

1 mol of H_2 molecules………contains: **6.02 x 10^{23}** H_2 molecules
2 x(6.02x10^{23}) H atoms

1 mol of **H_2O** molecules….contains: 6.02x10^{23} H_2O molecules
2 x (6.02x10^{23}) H atoms
1 x (6.02x10^{23}) O atoms

1 mol of Na^+ ions………..contains: **6.02 x 10^{23}** Na^+ ions

- The **atomic mass** of one atom expressed in **amu** is numerically the same as the **mass of one mole** of atoms of the element expressed in **grams**.

Element	Mass of one atom	Mass of one mole of atoms
H	1.008 amu	1.008 grams
Mg	24.31 amu	24.31 grams
Cl	35.45 amu	35.45 grams

MOLAR MASS

- The mass of one mole of a substance is called ***molar mass*** and is measured in ***grams***.

Mass of one mole of H_2O

$$\begin{array}{l} 2 \text{ mol H} = 2\,(1.008\text{ g}) = 2.02\text{ g} \\ 1 \text{ mol O} = 1\,(16.00\text{ g}) = \underline{16.00\text{ g}} \\ \qquad\qquad\qquad\qquad\qquad 18.02\text{ g} \end{array}$$

← **Molar Mass**

Mass of one mole of $Ca(OH)_2$

$$\begin{array}{l} 1 \text{ mol Ca} = 1\,(40.08\text{ g}) = 40.08\text{ g} \\ 2 \text{ mol O} = 1\,(16.00\text{ g}) = 32.00\text{ g} \\ 2 \text{ mol H} = 2\,(1.008\text{ g}) = \underline{2.02\text{ g}} \\ \qquad\qquad\qquad\qquad\qquad 74.10\text{ g} \end{array}$$

← **Molar Mass**

Examples:

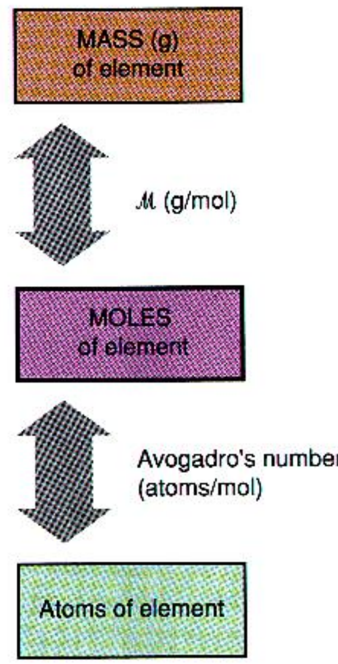
Calculate the molar mass of each compound shown below:

1. Lithium carbonate (Li_2CO_3)

2. Salicylic acid ($C_7H_6O_3$)

CALCULATIONS USING THE MOLE CONCEPT

When solving problems involving ***mass-mole-number*** relationships of elements or compounds, we can use:



- The ***molar mass*** to convert between mass and moles.
- ***Avogadro's number*** ($6.02\text{x}10^{23}$) to convert between moles and number of entities.

Examples:

1. How many **moles** of iron are present in 25.0 g of iron?

$$25.0 \text{ g Fe } \left(\frac{1 \text{ mole}}{55.85 \text{ g}}\right) = 0.448 \text{ mol Fe}$$

2. What is the mass of 5.00 mole of water?

3. How many magnesium **atoms** are present in 5.00 g of Mg?

$$5.00 \cancel{\text{ g}} \text{ Mg}\left(\frac{1 \cancel{\text{ mol}}}{24.3 \cancel{\text{ g}}}\right)\left(\frac{6.02\text{x}10^{23} \text{ atoms}}{1 \cancel{\text{ mol}}}\right) = 1.24\text{x}10^{23} \text{ atoms Mg}$$

4. How many molecules of HCl are present in 25.0 g of HCl?

MOLES OF ELEMENTS IN A FORMULA

- The subscripts in a chemical formula of a compound indicate the number of atoms of each type of element. For example, in a molecule of aspirin, $C_9H_8O_4$, there are 9 carbon atoms, 8 hydrogen atoms and 4 oxygen atoms.

- The subscript also indicates the number of moles of each element in one mole of the compound. For example, one mole of aspirin contains 9 moles of carbon atoms, 8 moles of hydrogen atoms and 4 moles of oxygen atoms.

$C_9H_8O_4$

	Carbon	**Hydrogen**	**Oxygen**
Atoms in 1 molecule	9 atoms C	8 atoms H	4 atoms O
Moles of atoms in 1 mole	9 moles C	8 moles H	4 moles O

- Using the subscripts from the aspirin formula, one can write the following conversion factors for each of the elements in 1 mole of aspirin:

$$\frac{\textbf{9 moles C}}{\textbf{1 mole } \mathbf{C_9H_8O_4}} \qquad \frac{\textbf{8 moles H}}{\textbf{1 mole } \mathbf{C_9H_8O_4}} \qquad \frac{\textbf{4 moles O}}{\textbf{1 mole } \mathbf{C_9H_8O_4}}$$

Examples:

1. Determine the moles of C atoms in 1 mole of each of the following substances:

   a) Acetaminophen used in Tylenol, $C_8H_9NO_2$

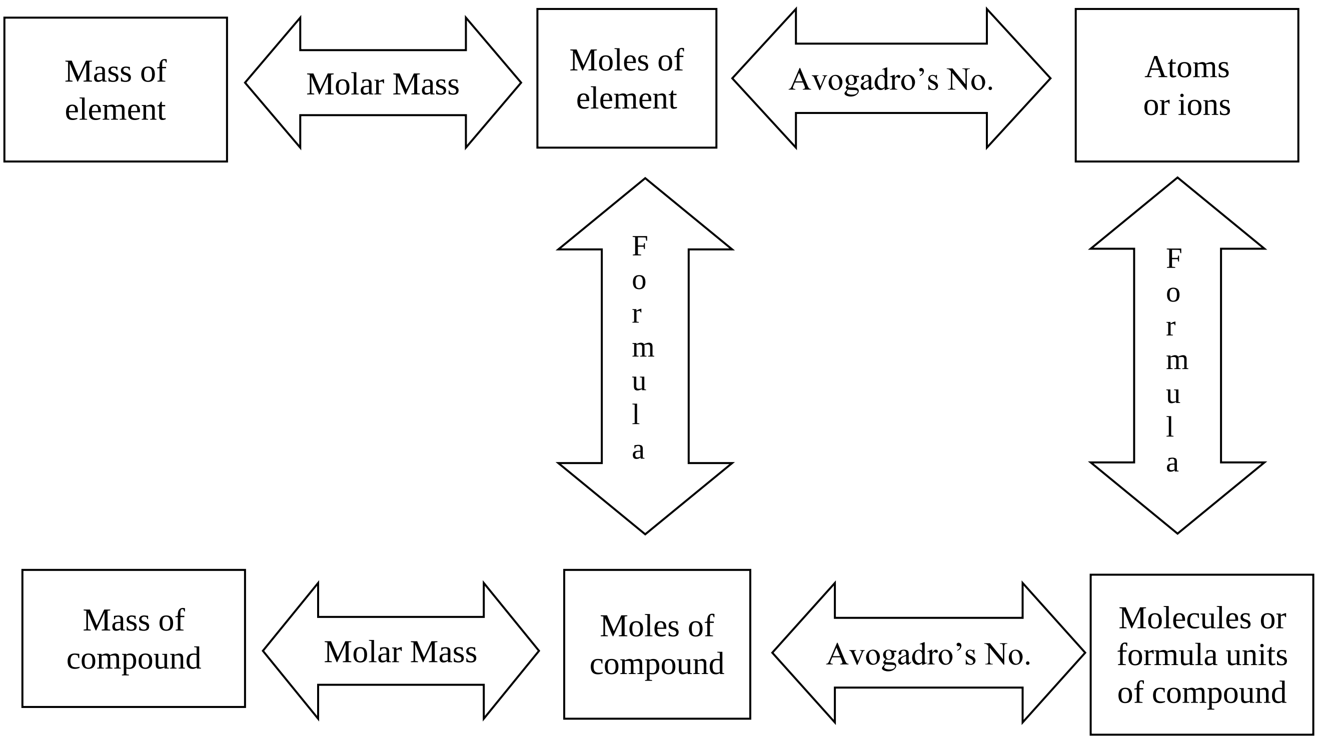
   b) Zinc dietary supplement, $Zn(C_2H_3O_2)_2$

2. How many carbon atoms are present in 1.50 moles of aspirin, $C_9H_8O_4$?

3. How many chlorine atoms are present in 15.0 g of CCl_4?

SUMMARY OF MASS-MOLE CALCULATIONS

Mass **Moles** **Particles**



Examples:

1. How many nitrogen atoms are present in 5.00 g of magnesium nitride?

2. How many phosphorus atoms are present in 1.00 g of calcium phosphate?

PERCENT COMPOSITION

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

$$\textbf{Mass \% X} = \frac{\textbf{(no. of X in formula) x (molar mass of X)}}{\textbf{molar mass of compound}} \textbf{ x 100}$$

Examples:

1. Determine the percent composition of K_2SO_4.

molar mass = 2(39.10 g)+1(32.06 g)+4(16.00 g)=
(78.20 g) + (32.06 g) + (64.00 g)=174.26 g

$$\% \text{ K} = \frac{78.20 \text{ g}}{174.26 \text{ g}} \text{x}100 = 44.86\%$$

$$\% \text{ S} = \frac{32.06 \text{ g}}{174.26 \text{ g}} \text{x}100 = 18.40\%$$

$$\% \text{ O} = \frac{64.00 \text{ g}}{174.26 \text{ g}} \text{x}100 = 36.73\%$$

2. 1.63 g of zinc combines with 0.40 g of oxygen to form zinc oxide. Determine the percent composition of the compound formed.

USING PERCENT COMPOSITION AS A CONVERSION FACTOR

- The mass percent composition of an element in a compound is a conversion factor between mass of the element and mass of the compound. For example, given that the mass percent of Cl in CCl_2F_2 is 58.64%, the following two conversion factors can be written:

$$\frac{58.64 \text{ g Cl}}{100 \text{ g } CCl_2F_2} \quad \text{or} \quad \frac{100 \text{ g } CCl_2F_2}{58.64 \text{ g Cl}}$$

Examples:

1. The FDA recommends that a person consume less than 2.4 g of sodium per day. How many grams of sodium chloride can a person consume and still be within this guideline? Sodium chloride is 39% sodium by mass.

2. What mass (in grams) of iron (III) chloride contains 58.2 g of iron?

DETERMINING EMPIRICAL FORMULAS

- Mass composition data can be used to determine the chemical formula of a compound. The formula obtained by this means is the empirical formula. The steps for this determination are listed below:

  1. Convert % composition data to mass by assuming 100 g of sample.
  2. Determine the mass of each element from data.
  3. Calculate the moles of each element from its mass
  4. Determine the smallest ratio between the moles of each element. If ratio is fractional, multiply by an integer till whole.

Examples:

1. Arsenic (As) reacts with oxygen (O) to form a compound that is 75.7% As and 24.3% oxygen by mass. What is the empirical formula for this compound?

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**

$$75.7\text{g As}\left(\frac{1\text{ mole}}{74.92\text{ g}}\right) = 1.01\text{ mol As}$$

$$24.3\text{ g O}\left(\frac{1\text{ mole}}{16.00\text{ g}}\right) = 1.52\text{ mol O}$$

Step 3. **Divide by small**

$$\text{As} = \frac{1.01\text{ mol}}{1.01\text{ mol}} = 1.00 \qquad \text{O} = \frac{1.52\text{ mol}}{1.01\text{ mol}} = 1.50$$

Step 4. **Multiply 'til whole**

$$\mathbf{As_{1.00}O_{1.50}\ \ x\ 2 = \boxed{As_2O_3}}$$

DETERMINING EMPIRICAL FORMULAS

- Empirical formula for a compound can also be calculated from experimental data on composition of compound. The steps for this determination are listed below:

  1. Determine the mass of each element from data.
  2. Calculate the moles of each element from its mass
  3. Determine the smallest ratio between the moles of each element. If ratio is fractional, multiply by an integer till whole.

Examples:

2. A sample of a compound is decomposed in the laboratory and found to contain 165 g of carbon, 27.8 g of hydrogen and 220.2 g of oxygen. Calculate the empirical formula of this compound.

3. A 3.24-g sample of titanium reacts with oxygen to form 5.40 g of the metal oxide. What is the formula of the metal oxide?

CALCULATING MOLECULAR FORMULA FROM EMPIRICAL FORMULA

- ***Molecular formula*** can be calculated from ***empirical formula*** if ***molar mass*** is known:

$$\text{Molecular formula} = (\text{empirical formula}) \times n$$

$$n\ (\text{multiplier}) = \frac{\text{molar mass}}{\text{mass of empirical formula}}$$

Examples:

1. A compound of N and O with a mass of 92.0 g has the empirical formula of NO_2. What is its molecular formula?

Mass of empirical formula =

1 N	14.01 g
2 O	<u>32.00 g</u>
	46.01 g

$$n = \frac{92.0\text{g}}{46.01\text{g}} = 2$$

Molecular formula = multiplier x empirical formula

$NO_2 \times 2 = N_2O_4$

2. Butane is a compound used as lighter fluid. Its empirical formula is C_2H_5 and its molar mass is 58.12 g/mol. Find the molecular formula for butane.

3. Caffeine, a stimulant found in coffee and soda, has the following mass percent composition: C, 49.48%; H, 5.19%; N, 28.85%; O, 16.48%. The molar mass of caffeine is 194.19 g/mol. Find the empirical and molecular formulas for caffeine.

4. Maleic acid is an organic compound composed of 41.39% C, 3.47% H, and the rest oxygen. If 0.129 mol of maleic acid has a mass of 15.0 g, what are the empirical and molecular formulas of maleic acid?