Reactions and Stoichiometry

Molecular mass: The sum of the atomic masses of all the atoms in a molecule of a substance.

Formula mass: The sum of the atomic masses of all the atoms in a formula unit of a substance.

For molecules: Molecular weight and formula weight are the same.

For ionic compounds: Only the term formula weight applies.

Mole: (mol)

One mole of a substance is the quantity of that substance that contains as many elemental entities as the number of atoms in exactly 12.000 g of Carbon-12.

That number is called Avogadro's number (N_A). It is numerically equal to 6.0221367×10^{23}.

A mole is just a counting number like a dozen or a ream or a pair.

When talking about a mole of something you must specify the formula unit of what you are using. 1 mol O is 6.022×10^{23} atoms of oxygen. 1 mol O_2 is 12.044×10^{23} atoms of oxygen.

Molar Mass: The mass of one mole of substance.

The molar mass in g/mol is numerically equivalent to the molecular or formula mass in amu.

Examples:

1. **How many formula units** are in 254.2 g of Lead(II) Oxide?

   The formula for Lead(II) Oxide is PbO which results in a molar mass of 223.19 g (207.19 g + 15.9994 g).

$$254.2\text{ g PbO}\times\frac{1\text{ mol PbO}}{223.19\text{ g PbO}}\times\frac{6.022\times10^{23}\text{ formula units PbO}}{1\text{ mol PbO}}=6.859\times10^{23}\text{ formula units PbO}$$

2. 3.42×10^{22} molecules of water has what **mass in grams**?

Water has the formula H_2O so it has a molar mass of 18.0153 g (2×1.0079 g + 15.9994 g).

$$3.42\times10^{22}\text{ molecules }H_2O\times\frac{1\text{ mole }H_2O}{6.022\times10^{23}\text{ molecules }H_2O}\times\frac{18.0153\text{ g }H_2O}{1\text{ mole }H_2O}=1.02\text{ g }H_2O$$

Mass percentages: The percentage by mass of all the elements in a compound.

$$\text{mass \% of A}=\frac{\text{mass of A in the sample}}{\text{mass of the sample}}\times100\%$$

The sum of the percentages for a compound must equal 100%.

Determining chemical formulas

Empirical formula: a formula for a compound that shows the lowest whole number ratio of the elements in the compound.

Empirical formula for water: H_2O
Empirical formula for hydrogen peroxide: HO (H_2O_2)
Empirical formula for glucose: CH_2O ($C_6H_{12}O_6$)
Empirical formula for ribose: CH_2O ($C_5H_{10}O_5$)

Determining the empirical formula from mass percentages…

1. Assume 100.00 g of compound. This converts the percentages directly to masses of the elements.

2. Convert the mass of each element to moles of that element.

3. Divide each of the moles by the smallest.

4. If you do not get a series of integers from step 3. Multiply each of the values by a factor to get everything to integers (±0.1). This factor will usually be about 2 or 3, but it may be larger.

Determining molecular formulas:

1. Find the empirical formula.

2. Find the empirical mass (the mass of one empirical formula unit).

3. Divide the molar mass by the empirical mass. This should be an integer.

4. Multiply this integer by all the subscripts in the formula.

For compounds containing the elements C, H, and O, the percentages can be determined by combustion. Combustion itself gives carbon dioxide, which gives the percentage of C, and water, which gives the percentage of H. Percentage of O is determined by difference.

Example:

A compound contains 62.04% C, 10.41% H, and the rest is Oxygen. What is the empirical formula for this compound?

Assume there is 100.00 g of the compound

$$100.00\,\text{g cpd} \times \frac{62.04\,\text{g C}}{100\,\text{g cpd}} \times \frac{1\,\text{mol C}}{12.011\,\text{g C}} = 5.165\,\text{mol C}$$

$$100.00\,\text{g cpd} \times \frac{10.41\,\text{g H}}{100\,\text{g cpd}} \times \frac{1\,\text{mol H}}{1.0079\,\text{g H}} = 10.32\,\text{mol H}$$

$$100.00\,\text{g cpd} \times \frac{27.55\,\text{g O}}{100\,\text{g cpd}} \times \frac{1\,\text{mol O}}{15.9994\,\text{g O}} = 1.722\,\text{mol O}$$

The smallest of these is 1.722 mol so we divide all the numbers by that one.

$$\frac{5.167\,\text{mol C}}{1.722\,\text{mol}} = 3.001 \approx 3$$

$$\frac{10.32\,\text{mol H}}{1.722\,\text{mol}} = 5.993 \approx 6$$

$$\frac{1.722\,\text{mol O}}{1.722\,\text{mol}} = 1.000 \approx 1$$

Therefore the empirical formula is C_3H_6O.

If the molar mass of this compound is 116.16 g mol^{-1}, what is the molecular formula?

$$\frac{\text{Molar mass}}{\text{Empirical mass}} = \frac{116.16\,\text{g mol}^{-1}}{58.08\,\text{g mol}^{-1}} = 2$$

So the molecular formula is twice the empirical formula, $C_6H_{12}O_2$.

Stoichiometry:

Molar interpretation vs. Molecular interpretation of a chemical reaction

The balanced chemical reaction gives you a series of conversion factors to use in problem solving.

$$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O$$

The conversion factors are obtained from the coefficients in the balanced chemical reaction. These conversion factors can be used to relate the amounts of reactant to other reactants or to amounts of products. It is this reason that, in order to solve a chemical problem, you first need to have a balanced chemical equation.

Example:

How many grams of solid Barium Sulfate can be produced from the reaction of 154.6 g of Barium Nitrate with Sodium Sulfate? The other product of the reaction is Sodium Nitrate.

First we need to write the balanced chemical equation:

$$Ba(NO_3)_2 + Na_2SO_4 \rightarrow BaSO_4 + 2\ NaNO_3$$

Now we can proceed with the calculation.

$$154.6\ \text{g Ba(NO}_3)_2 \times \frac{1\ \text{mol Ba(NO}_3)_2}{261.337\ \text{g Ba(NO}_3)_2} \times \frac{1\ \text{mol BaSO}_4}{1\ \text{mol Ba(NO}_3)_2} \times \frac{233.391\ \text{g BaSO}_4}{1\ \text{mol BaSO}_4} = 138.1\ \text{g BaSO}_4$$

Limiting Reactants

The **Limiting Reactant** is the reactant that is completely consumed during the course of a reaction. If the reactant is not completely consumed it is known as an **excess reactant**.

The limiting reactant is what determines the amount of product(s). When all of the limiting reactant is consumed, no more product(s) can be produced.

Determining the limiting reactant

1. Calculate the amount of product that would result from each of the reactants.

2. The reactant that corresponds to whichever amount of product is smallest is the limiting reactant. All other reactants are excess reactants.

Theoretical Yield is the maximum amount of product that can be produced from a reaction mixture. It is the amount of product determined from the limiting reactant.

Actual Yield is the amount of product that results when the reaction is carried out in the lab.

Percent yield is the ratio of actual yield to theoretical yield multiplied by 100.

$$\%\ \text{yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\%$$

Why determine the % yield? When a chemist reports his results from a reaction, he/she does so by using the percent yield. This is done because the percent yield should be the same for the same reaction regardless of how much reactant is initially used.

Example:

17.56 g of Ethanol (C_2H_6O) reacts with 102.5 g of Oxygen to produce Carbon Dioxide and water. How many grams of Carbon Dioxide are produced in this reaction? What is the limiting reactant? If only 30.00 g of Carbon Dioxide are produced, what is the percent yield?
Balanced Chemical Equation:

$$C_2H_6O + 3\ O_2 \rightarrow 2\ CO_2 + 3\ H_2O$$

Calculations:

$$17.56\ \mathrm{g\ C_2H_6O} \times \frac{1\ \mathrm{mol\ C_2H_6O}}{46.07\ \mathrm{g\ C_2H_6O}} \times \frac{2\ \mathrm{mol\ CO_2}}{1\ \mathrm{mol\ C_2H_6O}} \times \frac{44.01\ \mathrm{g\ CO_2}}{1\ \mathrm{mol\ CO_2}} = 33.54\ \mathrm{g\ CO_2}$$

$$102.5\ \mathrm{g\ O_2} \times \frac{1\ \mathrm{mol\ O_2}}{32.00\ \mathrm{g\ O_2}} \times \frac{2\ \mathrm{mol\ CO_2}}{3\ \mathrm{mol\ O_2}} \times \frac{44.01\ \mathrm{g\ CO_2}}{1\ \mathrm{mol\ CO_2}} = 93.98\ \mathrm{g\ CO_2}$$

$$\frac{30.00\ \mathrm{g\ CO_2}}{33.54\ \mathrm{g\ CO_2}} \times 100 = 89.45\%$$

The limiting reactant is the reactant that gives the smallest amount of product. In this case, that is Ethanol. The theoretical yield is that amount of product, 33.54 g CO_2. The percent yield is 89.45%.