Virtual Lab Manual

Stoichiometric Calculations: Identify an unknown compound using gravimetric analysis

Synopsis

Did you know that there are more water molecules in a glass of water than there are sand grains in the Sahara desert? In this simulation you will learn about the relationship between mass, molecular weight and the number of atoms or molecules and you will understand the magnitude and importance of Avogadro's number.

Identify an unknown compound

In order to identify a compound where the label has been partly destroyed, you must apply the technique of gravimetric analysis. To do so, you must first learn to understand the relationship between mass, moles and molecular weights and how to perform stoichiometric calculations from mass to mass via conversions to mole.

Stoichiometric calculations with moles

You will perform a realistic gravimetric analysis with detailed instructions on what to do and why to do it in every step of the experiment. From balancing the equation to recognizing the stoichiometry of the reactants and finding out which equation to employ in the calculations, the theory behind the experiment is explained step-by-step in the order of the experiment.

What compound is it?

At the end of the simulation, you will have finalized all of the stoichiometric calculations and the answer to the question should be clear... Can you see what compound it is?

Learning Objectives

At the end of this simulation, you will be able to...

- Explain the relationship between mass, molecular weight, and numbers of atoms or molecules and perform calculations deriving these quantities from one another
- Perform mass-to-mass stoichiometric calculations via conversions to mole
- Identify the limiting and excess reagents in a chemical reaction
- Calculate the theoretical, actual and percent reaction yield
- Define Avogadro's number and describe the mole quantification of matter

Techniques in Lab

- Gravimetric analysis

Theory

The Alkaline Earth Metals

The elements of the main group 2 of the periodic table are called the alkaline earth metals. The constituents of the group are Beryllium (Be), Magnesium (Mg), Calcium (Ca), Strontium (Sr), Barium (Ba) and Radium (Ra). Common for the elements of this group is that they are metals in their pure form, with low densities and low melting and boiling points. They all react with halides (F, Cl, Br, I) to form metal halides. Since the number of valence electrons of the alkaline earth metals is 2, the general formula of the formed metal halides is MX_2, where M is the metal and X is the halide.

All of the alkaline earth metals occur naturally, although Radon only occurs as a decay product from Uranium or Thorium, and is highly radioactive. Magnesium and Calcium are both among the top-8 most abundant elements on the earth's surface.

Balanced chemical equation

A chemical equation shows what happens in the chemical reaction. The basic chemical reaction can be written as follows:

Reactant → Product

Substance A + Substance B → Substance AB

In a balanced equation, the total number of atoms of each kind (e.g. A) in the reactants and products is the same.

The relationship between the different components of the reaction is referred to as the reaction stoichiometry.

Working example:
Unbalanced equation

$Na + O_2 \rightarrow Na_2O$

The reaction above, between sodium and oxygen, is not balanced. We need to adjust the number of units of some of the substances until we get equal numbers of each type of atom on both sides of the arrows.

Balanced equation

$4Na + O_2 \rightarrow 2Na_2O$

The equation is now balanced. Be sure to double check the number of atoms on the left side of the arrow matches the one on the right.

Gravimetric analysis
Gravimetric analysis is a technique to determine the amount of an analyte based on mass. A common example of a gravimetric analysis is to determine the amount of chloride in a solution - for example, to determine the amount of salt in seawater, or to determine the mass of the counter-ion of an unknown chloride compound. But the analyte could also be another ion.

The analyte is reacted with a counter-ion with which it forms an insoluble compound, which can then be isolated and weighed. From the mass of the precipitate the amount of the analyte can be calculated. If the analyte is the chloride ion, then the counter-ion could be silver, Ag^+, because AgCl is insoluble in water.

In order for the gravimetric analysis to be valid, we want all of the chloride ions to precipitate. This we obtain by letting chloride be the limiting reagent and the silver ions being in excess. In other words: There should be more silver ions than chloride ions. It is equally important that silver ion is introduced via a compound that is highly soluble in water so that the only precipitate is the silver chloride. The typical choice would be silver nitrate, $AgNO_3$:

$NaCl\ (aq) + AgNO_3\ (aq) \dashrightarrow Na^+\ (aq) + NO_3^-\ (aq) + AgCl\ (s)$

Moles and Avogadro's number
A mole is defined as the number of atoms present in 12 grams of ^{12}C. Since the atomic mass of ^{12}C is 12 amu, and 1 amu is 1.66×10^{-24} g, then 12 grams of ^{12}C must contain 6.022x1023 atoms:

$$\frac{12\ g}{12\ amu} = \frac{1\ g}{1\ amu} = \frac{1\ g}{1.66 \cdot 10^{-24}\ g} = 6.022 \cdot 10^{23}$$

This number is also referred to as Avogadro's number in recognition of the great Italian chemist Amedeo Avogadro.

It follows from this that since the mass of one atom of ^{12}C is 12 amu, then the mass of one mole of ^{12}C is 12 grams. The latter is called the molar mass and its unit is grams per mole (g/mol or $g \cdot mol^{-1}$). This is true for every atom in the periodic table: The mass stated in the periodic table is the mass of one atom in amu, but it is also the mass of one mole of those atoms in grams.

> **Examples:** The molar mass of Iron (Fe) is 55.845. It means that one atom of iron weighs 55.845 *amu* and that one mole of iron weighs 55.845 g. The molecular weight of water is 18.015. It means that one molecule of water weighs 18.015 *amu* and that one mole of water weighs 18.015 g.

Calculating molecular weights

The molecular weight Mw of a molecule can be found by adding the atomic weights of all the atoms that molecule is made of. Let's take Sulfuric Acid as an example. The formula of Sulfuric Acid is H2SO4. To calculate the molecular weight we take:

$$2 \cdot (\textit{atomic mass of } H) + (\textit{atomic mass of } S) + 4 \cdot (\textit{atomic mass of } O) =$$
$$2 \cdot 1.01\ amu + 32.06\ amu + 4 \cdot 16.00\ amu = 98.08\ amu$$

Just like the atomic mass in amu corresponds to the molar mass of that atom in grams, so the molecular weight of one molecule in amu corresponds to the molar mass in g/mol.

The relationship between M, m and n

The number of moles, n, of a substance can be found by using the following equation

> ***n(mol) = m(g) / M(g/mol)***

where m is the mass and M is the molecular weight of the given substance.

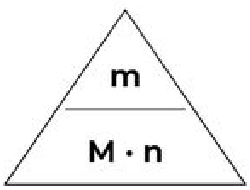
The molecular weight, M or Mw, is the mass in grams per one mole (g/mol or $g \cdot mol^{-1}$) of a substance. It can be calculated from the atomic weights of its constituent atoms, but when you look at the unit (g/mol) you can see that it can also be calculated if you know the mass of a substance (g) and how many moles that corresponds to (mol):

M(g/mol) = m(g)/ n(mol)

By rearranging this equation you can also calculate how many grams, a certain number of moles should weigh, by isolating m in the equation:

m(g) = n(mol) * M(g/mol)

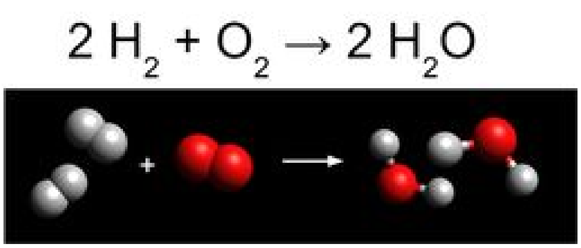
These three equations are very useful for many purposes in chemistry and it can be practical to find a mnemonic to memorize it. One way to do that is to write it up in a triangle like this:



When you cover the item you want to calculate, you have the equation written right there. You can remember that the little m should be at the top, because it looks like a bird which fly high above everything else.

Limiting and excess reagents

In the chemical equation where we form water from hydrogen and oxygen, we can see that hydrogen and oxygen reacts in a 2:1 ratio. This means that if you have two moles of hydrogen molecules and one mole of oxygen molecules, you have stoichiometric amounts of the reagents, and you form two moles of water.



But what if you only have one mole of hydrogen molecules? Then we say that hydrogen is the limiting reagent, and that we have an excess of oxygen. You can only form as much product as the limiting reagent, so in this case you can only form one mole of water molecules. When calculating the theoretical yield of your reacting, you have to take into account which is the limiting reagent.

Theoretical, experimental and percentage yield

The *theoretical yield* of a reaction is the amount of product you would get if you use up all of the limiting reagent, and if there is no loss, e.g. by degradation of reactant or product or by formation of byproducts. The *experimental yield* is the actual amount of product you obtain when performing a given experiment. The percentage yield is a calculation of how large a percentage of the theoretical yield you obtained in a given experiment. It is calculated by:

$$Percentage\ yield = \frac{experimental\ yield}{theoretical\ yield} \cdot 100\%$$

In most cases, when the yield of a reaction is mentioned without referring to either theoretical, experimental or percentage yield, it is implicitly the percentage yield that is meant.

Conversion between moles and molarity

When a compound is dissolved in a solvent the concentration of the compound is usually given in moles per liter (mol/l or mol·l^{-1}) which also called molarity, M. To calculate how large a volume, V, of a solution with a known concentration, c, to use in order to obtain a certain number of moles, n, the following equation is used:

$$V\ (L) = \frac{n\ (mol)}{c\ (mol/L)} \cdot 100\%$$

The equation can be rearranged to isolate for n or c if it should be desired.

Experimental thoroughness and accuracy

When performing chemical experiments in the laboratory a great deal of thoroughness and accuracy is necessary if you want to obtain reliable and reproducible results. It is important when you are performing a reaction that you measure accurate amounts of reactants to ensure the highest possible conversion, and thoroughness when you isolate your product, to minimize the loss and achieve the highest possible yield.

It is even more crucial when you are performing experiments within analytical chemistry. Here, sloppiness will not just lead to a poor yield, but can lead to a wrong conclusion to the analysis.

Below are some examples of things to be aware of:
- Contamination with other chemicals
- Causes for deviating yields

Suction filtration
- Place a rubber cone in the mouth of the suction flask.
- Place the Büchner funnel in the rubber cone.
- Place a filter paper inside the Büchner funnel.
- Turn on the vacuum.
- Pour a little of the solvent onto the filter to make it stick to the funnel.
- Pour the mixture to be filtered into the funnel.
- After all the liquid has been sucked through, wash the filter cake with at little solvent.