

Chemical equations and calculations

Basic chemical arithmetic and stoichiometry

A chemical equation expresses the net change in composition associated with a chemical reaction by showing the number of moles of reactants and products. But because each component has its own molar mass, equations also implicitly define the way in which the masses of products and reactants are related. In this unit we will concentrate on understanding and making use of these mass relations.

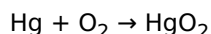
Yes, we are going to do a lot of "math" in this section, stuff you *must* know in order to master any respectable Chemistry course. But fear not, it's mostly Grade-4 arithmetic: simple proportionality and fractions. And even if you don't plan on doing any serious Chemistry later on, you will find the contents of this lesson an excellent review of these topics that will enable you to easily tackle any number of other numerical problems that come up again and again in everyone's life.

1 How to read and write chemical equations

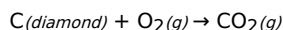
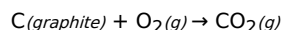
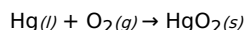
In a **chemical reaction**, one or more *reactants* are transformed into *products*:

reactants → products

The purpose of a **chemical equation** is to express this relation in terms of the formulas of the actual reactants and products that define a particular chemical change. For example, the reaction of mercury with oxygen to produce mercuric oxide would be expressed by the equation



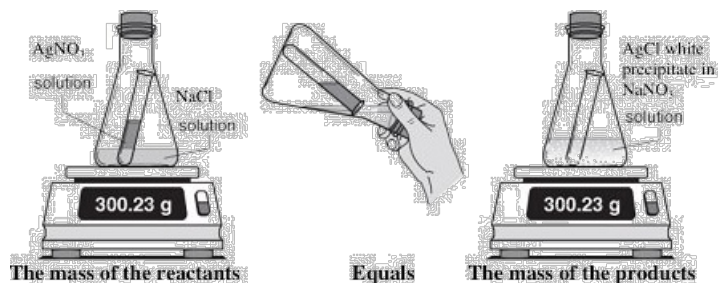
Sometimes, for convenience, it is desirable to indicate the physical state (gas, liquid or solid) of one or more of the species by appropriate abbreviations:



However, this is always optional.

Chemical equations *must* be balanced!

Basically, this means that chemical equations must be consistent with the *law of conservation of mass*:



In the context of an ordinary chemical reaction, conservation of mass means that atoms are neither created nor destroyed. This requirement is easily met by making sure that there are equal numbers of all atoms on both sides of the equation.

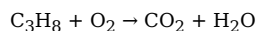
When we balance an equation, we simply make it consistent with the observed fact that individual atoms are conserved in chemical changes.

There is no set "recipe" for balancing ordinary chemical equations; it is best to begin by carefully studying selected examples such as those given below. For more detail, see the guidelines and examples in [Chapter 7](#) of Prof. Mark Bishop's excellent online textbook [Introduction to Chemistry](#)

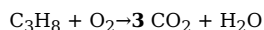
Problem Example 1: combustion of propane

Write a balanced equation for the combustion of propane C_3H_8 in oxygen O_2 . The products are carbon dioxide CO_2 and water H_2O .

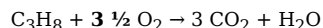
Solution: Begin by writing the unbalanced equation



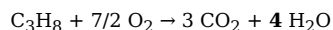
It is usually best to begin by balancing compounds containing the least abundant element, so we first balance the equation for carbon:



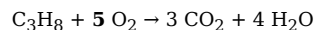
In balancing the oxygen, we see that there is no way that an even number of O_2 molecules on the left can yield the uneven number of O atoms shown on the right. Don't worry about this now— just use the appropriate fractional coefficient:



Finally, we balance the hydrogens by adding more waters on the right:



Ah, but now the oxygens are off again — fixing this also allows us to get rid of the fraction on the left side:

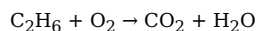


It often happens, however, that we do end up with a fractional coefficient, as in this variant of the above example.

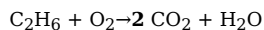
Problem Example 2: combustion of ethane

Write a balanced equation for the combustion of ethane C_2H_6 in oxygen O_2 . The products are carbon dioxide CO_2 and water H_2O .

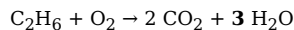
Solution: Begin by writing the unbalanced equation



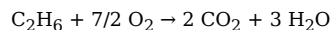
...then balance the carbon:



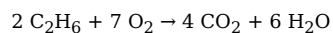
Let's balance the hydrogen next:



...but now we need a non-integral number of dioxygen molecules on the left:



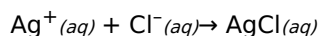
My preference is to simply leave it in this form; there is nothing wrong with $7/2 = 3 \frac{1}{2}$ moles of O_2 , and little to be gained by multiplying every term by two— not unless your teacher is a real stickler for doing it "by the book", in which case you had better write



2 Net ionic equations

Ionic compounds are usually dissociated in aqueous solution; thus if we combine solutions of silver nitrate AgNO_3 and sodium chloride NaCl we are really

combining four different species: the **cations** (positive ions) Ag^+ and Na^+ and the **anions** (negative ions) NO_3^- and Cl^- . It happens that when the ions Ag^+ and Cl^- are brought together, they will combine to form an insoluble precipitate of silver chloride. The net equation for this reaction is



Note that

- the ions NO_3^- and Cl^- are not directly involved in this reaction; the equation expresses only the *net change*, which is the removal of the silver and chloride ions from the solution to form an insoluble solid.
- the symbol (aq) signifies that the ions are in aqueous solution, and thus are *hydrated*, or attached to water molecules.
- the symbol (s) indicates that the substance AgCl exists as a solid. When a solid is formed in a reaction that takes place in solution, it is known as a **precipitate**. The formation of a precipitate is often indicated by underscoring.

Predicting the outcome when dissolved salts are mixed

From the above example involving silver chloride, it is clear that a meaningful net ionic equation can be written only if two ions combine to form an insoluble compound. In order to make this determination, it helps to know the *solubility rules*— which all students of chemistry were at one time required to memorize, but are nowadays usually obtained from tables such as the one shown below.

Anion (negative ion)	Cation (positive ion)	Soluble?
any anion	alkali metal ions (Li^+ , Na^+ , K^+ , etc.)	yes
nitrate, NO_3^-	any cation	yes
acetate, CH_3COO^-	any cation except Ag^+	yes
halide ions Cl^- , Br^- , or I^-	Ag^+ , Pb^{2+} , Hg_2^{2+} , Cu^{2+}	no
halide ions Cl^- , Br^- , or I^-	any other cation	yes
sulfate, SO_4^{2-}	Ca^{2+} , Sr^{2+} , Ba^{2+} , Ag^+ , Pb^{2+}	no
sulfate, SO_4^{2-}	any other cation	yes
sulfide, S_2^{2-}	alkali metal ions or NH_4^+	yes
sulfide, S_2^{2-}	Be^{2+} , Mg^{2+} , Ca^{2+} , Sr^{2+} , Ba^{2+} , Ra^{2+}	yes
sulfide, S_2^{2-}	any other cation	no
hydroxide, OH^-	alkali metal ions or NH_4^+	yes
hydroxide, OH^-	Sr^{2+} , Ba^{2+} , Ra^{2+}	slightly
hydroxide, OH^-	any other cation	no
phosphate, PO_4^{3-} , carbonate CO_3^{2-}	alkali metal ions or NH_4^+	yes
phosphate, PO_4^{3-} , carbonate CO_3^{2-}	any other cation	no

Problem Example 3: net ionic equations

Write net ionic equations for what happens when aqueous solutions of the following salts are combined:

- $\text{PbCl}_2 + \text{K}_2\text{SO}_4$
- $\text{K}_2\text{CO}_3 + \text{Sr}(\text{NO}_3)_2$
- $\text{AlCl}_3 + \text{CaSO}_4$
- $\text{Na}_3\text{PO}_4 + \text{CaCl}_2$

Solution: Use the solubility rules table (above) to find the insoluble combinations:

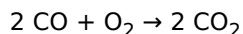
- $\text{Pb}^{2+}(\text{aq}) + \text{SO}_4^{2-}(\text{aq}) \rightarrow \text{PbSO}_4(\text{s})$
- $\text{Sr}^{2+}(\text{aq}) + \text{CO}_3^{2-}(\text{aq}) \rightarrow \text{SrCO}_3(\text{s})$
- no net reaction
- $3 \text{Ca}^{2+}(\text{aq}) + 2 \text{PO}_4^{3-}(\text{aq}) \rightarrow 3 \text{Ca}_3(\text{PO}_4)_2(\text{s})$

(Note the need to balance the electric charges)

3 Mass relations in chemical equations

Basic "chemical arithmetic"

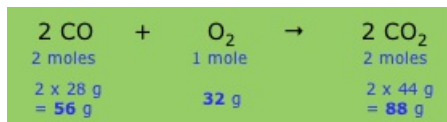
A balanced chemical equation expresses the relative number of moles of each component (product or reactant), but because each formula in the equation implies a definite mass of the substance (its molar mass), the equation also implies that certain weight relations exist between the components. For example, the equation describing the combustion of carbon monoxide to carbon dioxide



The term **stoichiometry** can refer to any type of calculation that relates the quantities of reactants and products in a chemical reaction. Stoichiometry is essentially an expression of the principle that atoms are *conserved* in chemical change.

The term comes from the Greek words στοιχείον *stoicheion* "element" and μέτρον *metron* "measure"

implies the following relations:



The relative masses shown in the bottom line establish the *stoichiometry* of the reaction, that is, the relations between the masses of the various components. Since these masses vary in direct proportion to one another, we can define what amounts to a conversion

factor (sometimes referred to as a *chemical factor*) that relates the mass of any one component to that of any other component.

Problem Example 4a: chemical factor and mass conversion

Evaluate the chemical factor and the conversion factor that relates the mass of carbon dioxide to that of the CO consumed in the reaction.

Solution: From the above box, the mass ratio of CO₂ to CO in this reaction is 88/56 = **1.57**; this is the *chemical factor* for the conversion of CO into CO₂.

The *conversion factor* is just 1.57/1, in which the mass units are explicitly stated:

(1.57 g CO₂ / 1 g CO)

But the same relation applies to any common set of mass or weight units, so we can simply say that the mass ratio of CO₂-to-CO expressed by the above equation is 1.57, which is also just the mass ratio of these two components in the equation. This, in turn, allows us to easily handle such problems as the following:

Problem Example 4b: mass-mass calculations in various units/span>

a) How many tons of CO₂ can be obtained from the combustion of 10 tons of CO?

b) How many kg of CO must be burnt to produce 20 kg of CO₂?

Solutions:

a) (1.57 T CO₂ / 1 T CO) × (10 T CO) = **15.7 T CO₂**

b) Notice the answer to this one must refer to carbon monoxide, not CO₂, so we write the conversion factor in reverse:

(1 kg CO / 1.57 kg CO₂) × (20 kg CO₂) = (20/1.57)g CO = **12.7 kg CO**.

Is this answer reasonable? Yes, because the mass of CO must always be smaller than that of CO₂ in this reaction.

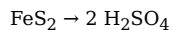
Mastering mass-mass problems

Don't expect to pass Chemistry unless you can handle problems such as the ones below; they come up frequently in all kinds of contexts. If you feel the need for more guidance, see one of the video tutorials listed near the bottom of this page.

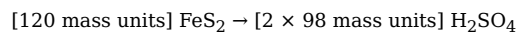
Problem Example 5

The ore FeS₂ can be converted into the important industrial chemical *sulfuric acid* H₂SO₄ by a series of processes. Assuming that the conversion is complete, how many liters of sulfuric acid (density 1.86 kg L⁻¹) can be made from 50 kg of ore?

Solution: As with most problems, this breaks down into several simpler ones. We begin by working out the stoichiometry on the assumption that all the sulfur in the ore ends up as H_2SO_4 , allowing us to write



Although this "skeleton" equation is incomplete (and thus not balanced), it *is* balanced in respect to the two components of interest, and this is all we need here. The molar masses of the two components are 120.0 and 98 g mol^{-1} , respectively, so the equation can be interpreted in terms of masses as



Thus 50 kg of ore will yield $(50 \text{ kg}) \times (196/120) = 81.7 \text{ kg}$ of product.

[*Check: is this answer reasonable? Yes, because the factor $(196/120)$ is close to $(200/120) = 5/3$, so the mass of product should be slightly smaller than twice the mass of ore consumed.*]

From the density information we find that the volume of liquid H_2SO_4 is

$$(81.7 \text{ kg}) \div (1.86 \text{ kg L}^{-1}) = \mathbf{43.9 \text{ L}}$$

[*Check: is this answer reasonable? Yes, because density tells us that the number of liters of acid will be slightly greater than half of its weight.*]

Problem Example 6

Barium chloride forms a crystalline hydrate, $\text{BaCl}_2 \cdot x\text{H}_2\text{O}$, in which x molecules of water are incorporated into the crystalline solid for every unit of BaCl_2 . This water can be driven off by heat; if 1.10 g of the hydrated salt is heated and reweighed several times until no further loss of weight (i.e., loss of water) occurs, the final weight of the sample is 0.937 g. What is the value of x in the formula of the hydrate?

Solution:

The first step is to find the number of moles of BaCl_2 (molecular weight 208.2) from the mass of the dehydrated sample.

$$(0.937 \text{ g}) / (208.2 \text{ g mol}^{-1}) = 0.00450 \text{ mol}$$

Now find the moles of H_2O (molecular weight 18) lost when the sample was dried:

$$(1.10 - .937)\text{g} / (18 \text{ g mol}^{-1}) = .00905 \text{ mol}$$

Allowing for a reasonable amount of measurement error, it is apparent that the mole ratio of $\text{BaCl}_2 \cdot \text{H}_2\text{O} = 1:2$. The formula of the hydrate is **$\text{BaCl}_2 \cdot 2\text{H}_2\text{O}$** .

4 Understanding limiting reactants

Most chemical reactions that take place in the real world begin with more or less arbitrary amounts of the various reactants; we usually have to make a special effort if we want to ensure that stoichiometric amounts of the reactants are combined. This means that one or more reactant will usually be present in excess; there will be more present than can react, and some will remain after the reaction is over. At the same time, one reactant will be completely used up; we call this the **limiting reactant** because the amount of this substance present will control, or limit, the quantities of the other reactants that are consumed as well as the amounts of products produced.

Limiting reactant problems are handled in the same way as ordinary stoichiometry problems with one additional preliminary step: you must first determine which of the reactants is limiting— that is, which one will be completely used up. To start you off, consider the following very simple example

Problem Example 7

For the hypothetical reaction **$3 \text{ A} + 4 \text{ B} \rightarrow [\text{products}]$** , determine which reactant will be completely consumed when we combine

- a) equimolar quantities of A and B;
- b) 0.57 mol of A and 0.68 mol of B.

Solution:

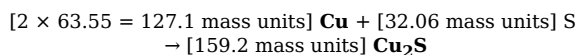
a) Simple inspection of the equation shows clearly that more moles of B are required, so this component will be consumed (and is thus the limiting reactant), leaving behind $\frac{3}{4}$ as many moles of A.

b) How many moles of B will react with .57 mol of A? The answer will be $(4/3 \times 0.57 \text{ mol})$. If this comes to less than 0.68 mol, then B will be the limiting reactant, and you must continue the problem on the basis of the amount of B present. If the limiting reactant is A, then all 0.57 mol of A will react, leaving some of the B in excess. Work it out!

Problem Example 8

Sulfur and copper, when heated together, react to form copper(I) sulfide, Cu_2S . How many grams of Cu_2S can be made from 10 g of sulfur and 15 g of copper?

Solution: From the atomic weights of Cu (63.55) and S (32.06) we can interpret the reaction $2\text{Cu} + \text{S} \rightarrow \text{Cu}_2\text{S}$ as



Thus 10 g of S will require $(10 \text{ g S}) \times (127.1 \text{ g Cu}) / (32.06 \text{ g S}) = 39.6 \text{ g Cu}$...which is a lot more than what is available, so **copper is the limiting reactant** here.

[Check: is this answer reasonable? Yes, because the chemical factor (127/32) works out to about 4, indicating that sulfur reacts with about four times its weight of copper.]

The mass of copper sulfide formed will be determined by the mass of copper available:

$$(15 \text{ g Cu}) \times (159.2 \text{ g Cu}_2\text{S}) / (127.1 \text{ g Cu}) = \mathbf{18.8 \text{ g Cu}_2\text{S}}$$

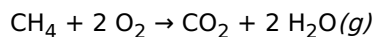
[Check: is this answer reasonable? Yes, because the chemical factor (159.2/127.1) is just a bit greater than unity, indicating that the mass of the product will slightly exceed that of the copper consumed.]

Limiting reactants in everyday life

The concept of limiting reactants touches us all in our everyday lives — and as we will show in the second example below, even in the maintenance of life itself!

Air-to-fuel ratios in combustion

Combustion is an exothermic process in which a fuel is combined with oxygen; *complete* combustion of a hydrocarbon fuel such as methane or gasoline yields carbon dioxide and water:

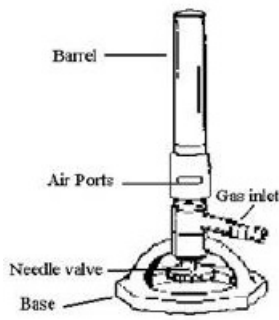


Problem Example 9: fuel-to-oxygen mass ratio in combustion of methane

Calculate the mass ratio of CH_4 to O_2 required for complete combustion.

Solution: This is just the ratio of the molar mass of CH_4 (16 g) to that of two moles of dioxygen (2 x 32 g)

Thus $(64 \text{ g}) / (16 \text{ g}) = 4/1 = \mathbf{4.0}$.



Complete combustion of each kg of methane consumes 4 kg of dioxygen, which is supplied by the air. In the classic Bunsen burner, this air is admitted through an adjustable opening near the base. When it is fully open, the flame is blue in color and achieves its maximum



temperature, indicating that combustion is approximately stoichiometric. If the opening is gradually closed, the appearance of the flame changes as illustrated. Under these conditions, oxygen becomes the limiting reactant and combustion is incomplete.

Incomplete combustion is generally undesirable because it wastes fuel, produces less heat, and releases pollutants such as carbon soot. Energy-producing combustion processes should always operate in fuel-limited mode.

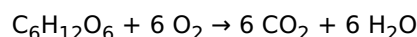
In ordinary combustion processes, the source of oxygen is air. Because only about 20 percent of the molecules in dry air consist of O_2 , the volume of air that must be supplied is five times greater than what would be required for pure O_2 . Calculation of the *air-to-fuel mass ratio* ("A/F ratio") employed by combustion engineers is complicated by the differing molar masses of dioxygen and air. For methane combustion, the A/F ratio works out to about 17.2. A/F ratios which exceed the stoichiometric values are said to be *lean*, while those in which air becomes the limiting component are characterized as *rich*. In order to ensure complete combustion, it is common practice to maintain a slightly lean mixture. The quantities of so-called *excess air* commonly admitted to burners vary from 5-10% for natural gas to up to 100% for certain grades of coal.

For internal combustion engines fueled by gasoline (roughly equivalent to C_7H_{14}), the stoichiometric A/F ratio is 15:1. However, practical considerations necessitate differing ratios at various stages of operation. Typical values vary from a rich ratio for starting or acceleration to slightly lean ratios for ordinary driving. These ratios are set by the *carburetor*, with additional control by the engine computer and exhaust-line oxygen sensor in modern vehicles, or by a manual *choke* in earlier ones.

Aerobic and anaerobic respiration

Our bodies require a continual supply of energy in order to maintain neural activity, synthesize proteins and other essential biochemical components, replace cells, and to power muscular action. The "fuel" — the carrier of chemical energy — glucose, a simple sugar which is released as needed from the starch-like polymer glycogen, the form in which the energy we derive from food is stored.

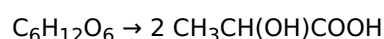
Arterial blood carries dissolved glucose along with hemoglobin-bound dioxygen to individual cells which are the sites of glucose "combustion":



The net reaction and the quantity of energy released are the same as if the glucose were burned in the open air, but within the cells the reaction proceeds in a series of tiny steps which capture most of this energy for the body's use, liberating only a small fraction of it as thermal energy (heat).

Because this process utilizes oxygen from the air we breath, it is known as **aerobic respiration**. And as with any efficient combustion process, glucose is the limiting reactant here.

But there are times when vigorous physical activity causes muscles to consume glucose at a rate that exceeds the capacity of the blood to deliver the required quantity of oxygen. Under these conditions, cellular respiration shifts to an alternative **anaerobic** mode:



As you can see from this equation, glucose is only partially broken down (into

lactic acid), and thus only part of its chemical energy is captured by the body.



There are numerous health benefits to aerobic exercise, including increased ability of the body to maintain an aerobic condition. But if you are into short-distance running (sprinting) or being pursued by a tiger, the reduced efficiency of anaerobic exercise may be a small price to pay.



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