Equations and Mass Relationships in Physics

It's fairly easy to synthesize a superconductor, but to do so, you need to understand the principles of "stoichiometry". This is surprising, because superconductors are often materials that are considered "non-stoichiometric" berthollides[1]. We'll explain below.

Superconductivity results in the famous Meissner Effect shown in the Figure or on YouTube. The effect is due to the expulsion of magnetic fields by superconductors, so they become perfectly diamagnetic[2]. Superconductivity can be measured by the standard technique shown in the Figure, where the measured voltage drops to zero when the pellet is cooled below the "critical temperature".

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The "1-2-3 Superconductor" the Bednorz and Müller synthesized may be the best known. It gets its name from its formula, YBa$_2$Cu$_3$O$_{7-x}$, which shows that it contains 1 atom of Yttrium, 2 of barium, and 3 of copper. The number of oxygen atoms, "7-x", is variable, making the compound "nonstoichiometric", but stoichiometric principles are still necessary for its synthesis. The oxygen content depends on the atmosphere above the compound at various stages in its synthesis. The highest temperature superconductor is found for x = 0.15, where the "critical temperature", where superconductivity commences, is Tc = 92 K or -181 °C, and superconductivity disappears at x ≈ 0.6.

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Present and Future Uses of Superconductors

Superconducting magnets are used in MRI and NMR machines, mass spectrometers, and in particle accelerators to focus particle beams. They are the building blocks of SQUIDs (superconducting quantum interference devices), the most
sensitive magnetometers known. They may be used in advanced transportation, for efficient electric motors and magnetic levitation devices [3]. The 1987 Nobel prize was awarded to Bednorz and Müller at IBM Zurich for their discovery of superconductivity in copper containing oxides at over 30 K, and the search for higher temperature superconductors has been intense since that time.

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**Synthesis of a Superconductor**

The 1-2-3 superconductor may be synthesized[4] by mixing 0.60 g of yttrium oxide with "stoichiometric quantities" (see below) of barium peroxide and copper (II) oxide according to the equation:

\[
\text{2Y}_2\text{O}_3 + 8\text{BaO}_2 + 12\text{CuO} \rightarrow 4 \text{YBa}_2\text{Cu}_3\text{O}_6 + 5 \text{O}_2
\]

The YBa\(_2\)Cu\(_3\)O\(_{7-x}\) is prepared by grinding the reactants together, strongly heating "calcinating" at 900–950 °C for 8-12 hours, pelletizing the powder mixture, heating or "sintering" the pellet at 950 °C for 12 or more hours, then maintaining the product at 500°C for 12-16 hours. On slow cooling in oxygen atmosphere, YBa2Cu3O6 is converted to nonstoichiometric, superconducting YBa2Cu3O7-x forms by uptake and loss of oxygen[5].

But what does the phrase "stoichiometric quantities" in the procedure above mean?

A balanced chemical equation such as Equation 1 not only tells how many molecules of each kind are involved in a reaction, it also indicates the amount of each substance that is involved. Equation (1) says that 2 \(\text{Y}_2\text{O}_3\) formula units can react with 8 \(\text{BaO}_2\) formula units and 12 \(\text{CuO}\) formula units to give 4 \(\text{YBa}_2\text{Cu}_3\text{O}_6\) formula Units and 5 \(\text{O}_2\) molecules. Here we've used the term "formula unit" to indicate that the substance may not be a molecule, but rather an ionic compound or "network crystal". A "formula unit" gives the composition of the substance without specifying the type of bonding.

Eq. (1) also says that 2 mol \(\text{Y}_2\text{O}_3\) reacts with 8 mol \(\text{BaO}_2\) and 12 mol \(\text{CuO}\) yielding 4 mol \(\text{YBa}_2\text{Cu}_3\text{O}_6\) and 5 mol \(\text{O}_2\).

The balanced equation does more than this, though. It also tells us that \(2 \times 4 = 8\) mol \(\text{Y}_2\text{O}_3\) will react with \(2 \times 8 = 16\) mol \(\text{BaO}_2\) and \(2 \times 12 = 24\) mol \(\text{BaO}_2\), and \(2 \times 12 = 24\) mol \(\text{CuO}\) to give \(2 \times 4 = 8\) mol \(\text{YBa}_2\text{Cu}_3\text{O}_6\) and \(2 \times 5 = 10\) mol \(\text{O}_2\).

It also tells us that \(\frac{1}{2} \times 4 = 2\) mol \(\text{Y}_2\text{O}_3\) requires only \(\frac{1}{2} \times 8 = 4\) mol \(\text{BaO}_2\) and \(\frac{1}{2} \times 12 = 6\) mol \(\text{CuO}\), to give \(\frac{1}{2} \times 4 = 2\) mol \(\text{YBa}_2\text{Cu}_3\text{O}_6\) and \(\frac{1}{2} \times 5 = 2.5\) mol \(\text{O}_2\). In other words, the equation indicates that exactly 8 mol \(\text{BaO}_2\) must react for every 2 mol \(\text{Y}_2\text{O}_3\) consumed. For the purpose of calculating how much \(\text{BaO}_2\) is required to react with a certain amount of \(\text{Y}_2\text{O}_3\) therefore, the significant information contained in Eq. (1) is the ratio

\[
\frac{8 \text{ mol BaO}_2}{2 \text{ mol Y}_2\text{O}_3} = \frac{2 \text{ mol Y}_2\text{O}_3}{4 \text{ mol BaO}_2} = \frac{2 \text{ mol Y}_2\text{O}_3}{1 \text{ mol CuO}} = \frac{1 \text{ mol CuO}}{2 \text{ mol Y}_2\text{O}_3}
\]

We shall call such a ratio derived from a balanced chemical equation a **stoichiometric ratio** and give it the symbol \(S\). Thus, for Eq. (1),
The word **stoichiometric** comes from the Greek words *stoicheion*, “element,” and *metron*, “measure.” Hence the stoichiometric ratio measures one element (or compound) against another.

**Example (PageIndex{1}): Stoichiometric Ratio**

Derive 4 additional stoichiometric ratios from Eq. \(\text{(ref{1})}\)

**Solution:** Any ratio of amounts of substance given by coefficients in the equation may be used:

\[ \frac{\text{S}(\frac{\text{BaO}_2}{\text{Y}_2\text{O}_3})}{\text{8 mol BaO}_2}{\text{2 mol Y}_2\text{O}_3}}{\text{(2)}} \]

\[ \frac{\text{S}(\frac{\text{Y}_2\text{O}_3}{\text{O}_2})}{\text{2 mol Y}_2\text{O}_3}{\text{5 mol O}_2}} \]

\[ \frac{\text{S}(\frac{\text{O}_2}{\text{CuO}})}{\text{5 mol O}_2}{\text{12 mol CuO}}} \]

\[ \frac{\text{S}(\frac{\text{Y}_2\text{O}_3}{\text{CuO}})}{\text{2 mol Y}_2\text{O}_3}{\text{12 mol CuO}}} \]

\[ \frac{\text{S}(\frac{\text{O}_2}{\text{YBa}_2\text{Cu}_3\text{O}_6})}{\text{5 mol O}_2}{\text{4 mol YBa}_2\text{Cu}_3\text{O}_6}}} \]

There are several more stoichiometric ratios, each connecting any two reactants or products.

When any chemical reaction occurs, the amounts of substances consumed or produced are related by the appropriate stoichiometric ratios. Using Eq. (1) as an example, this means that the ratio of the amount of BaO\(_2\) consumed to the amount of Y\(_2\)O\(_3\) consumed must be the stoichiometric ratio S(BaO\(_2\)/Y\(_2\)O\(_3\)):

\[ \frac{n_\text{BaO}_2\text{ consumed}}{n_\text{Y}_2\text{O}_3\text{ consumed}} = \text{S}(\frac{\text{BaO}_2}{\text{Y}_2\text{O}_3}) = \frac{8 \text{ mol BaO}_2}{2 \text{ mol Y}_2\text{O}_3} \]

Similarly, the ratio of the amount of YBa\(_2\)Cu\(_3\)O\(_6\) produced to the amount of Y\(_2\)O\(_3\) consumed must be

S(YBa\(_2\)Cu\(_3\)O\(_6\)/Y\(_2\)O\(_3\)):

\[ \frac{n_\text{YBa}_2\text{Cu}_3\text{O}_6\text{ produced}}{n_\text{Y}_2\text{O}_3\text{ consumed}} = \text{S}(\frac{\text{YBa}_2\text{Cu}_3\text{O}_6}{\text{Y}_2\text{O}_3}) = \frac{4 \text{ mol YBa}_2\text{Cu}_3\text{O}_6}{2 \text{ mol Y}_2\text{O}_3} \]
In general we can say that

\[ \text{Stoichiometric ratio } \left( \frac{X}{Y} \right) = \frac{\text{amount of X consumed or produced}}{\text{amount of Y consumed or produced}} \] (3a)

or, in symbols,

\[ \text{S} \left( \frac{X}{Y} \right) = \frac{n_{\text{X consumed or produced}}}{n_{\text{Y consumed or produced}}} \] (3b)

Note

Note that in the word Eq. (3a) and the symbolic Eq. (3b), X and Y may represent any reactant or any product in the balanced chemical equation from which the stoichiometric ratio was derived. No matter how much of each reactant we have, the amounts of reactants consumed and the amounts of products produced will be in appropriate stoichiometric ratios.

**Example**: Amount of Product

Find the amount of YBa$_2$Cu$_3$O$_6$ produced when 3.68 mol Y$_2$O$_3$ is consumed according to Eq. 1.

**Solution**: The amount of YBa$_2$Cu$_3$O$_6$ produced must be in the stoichiometric ratio S(YBa$_2$Cu$_3$O$_6$//Y$_2$O$_3$) to the amount of Y$_2$O$_3$ consumed:

\[ \text{S} \left( \frac{\text{YBa}_{2}\text{Cu}_{3}\text{O}_{6}}{\text{Y}_{2}\text{O}_{3}} \right) = \frac{n_{\text{YBa}_{2}\text{Cu}_{3}\text{O}_{6} \text{ produced}}}{n_{\text{Y}_{2}\text{O}_{3} \text{ consumed}}} \]

Multiplying both sides $n_{\text{Y}_2\text{O}_3 \text{ consumed}}$, by we have

\[ n_{\text{Y}_2\text{O}_3 \text{ consumed}} \times \text{S} \left( \frac{\text{YBa}_{2}\text{Cu}_{3}\text{O}_{6}}{\text{Y}_{2}\text{O}_{3}} \right) = 3.68 \text{ mol Y}_2\text{O}_3 \times \frac{4 \text{ mol YBa}_{2}\text{Cu}_{3}\text{O}_{6}}{2 \text{ mol Y}_{2}\text{O}_{3}} = 7.36 \text{ mol YBa}_{2}\text{Cu}_{3}\text{O}_{6} \]

This is a typical illustration of the use of a stoichiometric ratio as a conversion factor. Example 2 is analogous to Examples 1 and 2 from Conversion Factors and Functions, where density was employed as a conversion factor between mass and
volume. Example 2 is also analogous to Examples 2.4 and 2.6, in which the Avogadro constant and molar mass were used as conversion factors. As in these previous cases, there is no need to memorize or do algebraic manipulations with Eq. (3) when using the stoichiometric ratio. Simply remember that the coefficients in a balanced chemical equation give stoichiometric ratios, and that the proper choice results in cancellation of units. In road-map form

\[ n_{\text{X consumed or produced}} \xrightarrow{S(\text{X/Y})} n_{\text{Y consumed or produced}} \]

When using stoichiometric ratios, be sure you *always* indicate moles of what. You can only cancel moles of the same substance. In other words, 1 mol \( Y_2O_3 \) cancels 1 mol \( Y_2O_3 \) but does not cancel 1 mol \( YBa_2Cu_3O_6 \).

The next example shows that stoichiometric ratios are also useful in problems involving the mass of a reactant or product.

**Example \( \PageIndex{3} \) : Mass Required**

Calculate the mass of BaO\(_2\) required when 3.68 mol \( Y_2O_3 \) is consumed according to Equation \( \ref{1} \).

**Solution:** The problem asks that we calculate the mass of BaO\(_2\) consumed. As we learned in *Example 2 of The Molar Mass*, the molar mass can be used to convert from the amount of BaO\(_2\) to the mass of BaO\(_2\). Therefore this problem in effect is asking that we calculate the amount of BaO\(_2\) consumed from the amount of \( Y_2O_3 \) consumed. This is the same kind of problem as in Example 2. It requires the stoichiometric ratio

\[ \left( \frac{\text{BaO}_2}{\text{Y}_2\text{O}_3} \right) = \frac{8 \text{ mol BaO}_2}{2 \text{ mol Y}_2\text{O}_3} \]

The amount of BaO\(_2\) consumed is then

\[ n_{\text{BaO}_2 \text{ consumed}} = n_{\text{Y}_2\text{O}_3 \text{ consumed}} \times \text{conversion factor} \approx 3.68 \text{ mol Y}_2\text{O}_3 \times 8 \text{ mol BaO}_2 \times \frac{169.33 \text{ g BaO}_2}{1 \text{ mol BaO}_2} \]

The mass of BaO\(_2\) is

\[ m_{\text{BaO}_2} = 14.72 \text{ mol BaO}_2 \times 169.33 \text{ g BaO}_2 = 2493 \text{ g BaO}_2 \]

With practice this kind of problem can be solved in one step by concentrating on the units. The appropriate stoichiometric
ratio will convert moles of Y$_2$O$_3$ to moles of Y$_2$O$_3$ and the molar mass will convert moles of BaO$_2$ to grams of BaO$_2$. A schematic road map for the one-step calculation can be written as

\[
\underbrace{n_{\text{Y}_2\text{O}_3}}_{\text{(S\text{BaO}_2/\text{Y}_2\text{O}_3)}} \underbrace{n_{\text{BaO}_2}}_{\text{(M\text{BaO}_2/\text{BaO}_2}}} \underbrace{m_{\text{BaO}_2}}_{\text{ice(BaO2)}}
\]

Thus

\[
\underbrace{\text{m}_{\text{BaO}_2}}_{\text{ice(BaO2)}} = \underbrace{\text{3.68 mol Y}_2\text{O}_3}_{\text{(S\text{BaO}_2/\text{Y}_2\text{O}_3)}} \times \underbrace{\frac{\text{8 mol BaO}_2}{\text{2 mol Y}_2\text{O}_3}}_{\text{(M\text{BaO}_2/\text{BaO}_2}}} \times \underbrace{\frac{169.33 \text{ g}}{\text{1 mol BaO}_2}}_{\text{ice(BaO2)}} = 1.56 \text{g } \ce{BaO2}
\]

These calculations can be organized as a table, with entries below the respective reactants and products in the chemical equation. You may verify the additional calculations.

| 2 Y$_2$O$_3$ + 8 BaO$_2$ + 12 CuO → 4 YBa$_2$Cu$_3$O$_6$ + 5 O$_2$ |
|-----------------|----------------|-----------------|----------------|----------------|
| m (g) | 831.0 | 2493 | 1757 | 4786 | 294.4 |
| M (g/mol) | 225.81 | 169.33 | 79.55 | 650.2 | 32 |
| n (mol) | 3.68 | 14.72 | 22.08 | 7.36 | 9.20 |

Example $\PageIndex{4}$: Mass of Reactants

The highest temperature superconductor synthesized so far is HgBa$_2$Ca$_2$Cu$_3$O$_{8+x}$ with $T_c = 134$ K.

Although the synthesis is more complicated$^6$$^7$ then the one above, we can explore the stoichiometry, as usual, by writing an equation for the synthesis of the stoichiometric compound HgBa$_2$Ca$_2$Cu$_3$O$_8$. The stoichiometric compound is heated in oxygen to produce the nonstoichiometric superconductor.

HgO + 2 BaO$_2$ + 2 CaO + 3 CuO → HgBa$_2$Ca$_2$Cu$_3$O$_8$ + O$_2$

Prepare a table like the one above, calculating the amount and mass of each reactant necessary to consume 1 g of HgO, and the amount and mass of products formed.

Solution:

The problem gives the mass of HgO and asks for the amounts and masses of other reactants and products. Thinking the
problem through before trying to solve it, we realize that the molar mass of HgO could be used to calculate the amount of HgO consumed. Then we need stoichiometric ratios to get the amounts of other reactants and products. Finally, the molar masses of permit calculation of the masses. Symbolically, for the reactant BaO₂,

\[
\begin{align*}
0.00462 &\quad 0.00923 &\quad 0.00923 &\quad 0.0139 &\quad 0.00462 &\quad 0.00462 \\
\end{align*}
\]

Make sure you can do these calculations, and show that the sum of the masses of the reactants equals the sum of the masses of products as a final check.

From ChemPRIME: 3.1: Equations and Mass Relationships

References

4. ↑ http://materials.binghamton.edu/labs...er/superc.html

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