Introduction

Chemical formulas tell us what kind of elements are in a compound. They also tell us the number of each type of element in a **formula unit**.

For example, the formula $(NH_4)_2SO_4$ would tell us that each formula unit of ammonium sulfate contains **two** N atoms, **eight** H atoms, **one** S atom, and **four** O atoms. The subscripts in chemical formulas are also good for **moles** of atoms. After all, they are ratios between the atoms. A ratio of 1:2 is the same thing as a ratio of 2:4 is the same thing as a ratio of 6.022×10^{23}:12.044×10^{23}!

So what? What can we do with a chemical formula alone? This note pack will tell you a few things you can do with a chemical formula.

Applications of chemical formulas: Mass percentages from a formula

The chemical formula tells you about the makeup, or composition, of something. Sometimes you're interested in the composition of a chemical:

1. Farmers might be interested in how much nitrogen is in their fertilizer.
2. The health conscious might be interested in how much "sodium" they're really putting on their food when they add table salt to it.
3. It's often easy (in a lab) to find the elemental makeup of a chemical compound - expressed as the mass percentage of each element the compound contains . The percentages can be used to help identify the compound.

If you are dealing with a pure substance and know its chemical formula, a little math will give you the percentage of each element in the compound.

Let's take the first example - nitrogen in a fertilizer. *Ammonium nitrate, NH_4NO_3, can be used as a fertilizer. Let's say we want to find out how much nitrogen is in the fertilizer. Since we can weigh out fertilizer by weight (mass), we'd like to know the percent by mass of nitrogen.*

Given: NH_4NO_3 **Find: %N (by mass) in NH_4NO_3**

The chemical formula of a compound tells us about the ratio of moles of elements in a given amount of compound. Moles can be easily related to mass via the **formula weight**.

So, we can calculate the **MASS RATIO** from the **MOLE RATIO** in the chemical formula!

Assume you have **exactly one** mole of the substance. Since we are calculating a ratio, it doesn't mathematically matter what number of moles we assume: 1, 12, 42, 6.022×10^{23}, etc. Assuming one mole, though, makes the calculations easiest.

In **one** mole of ammonium nitrate, there are **two** moles of nitrogen. (NH_4NO_3) So, convert two moles of nitrogen to grams using the formula weight of N (**the atomic weight**):

$$2\ \text{mol N} \times \frac{14.00674\ \text{g N}}{1\ \text{mol N}} = 28.01348\ \text{g N}$$

To find the percent nitrogen by mass we need to compare this weight to the **total** weight of a mole of ammonium nitrate. The mass of one mole of any compound is given by its **formula weight**. The formula weight of ammonium nitrate is 80.0434 g/mol.

$$\text{Percentage N by mass} = \frac{28.01348\ \text{g N}}{\mathbf{80.0434\ g\ total}} \times 100\% = 35.00\%\ \text{N by mass}$$

So, the ammonium nitrate contains 35.00% nitrogen by mass.

Prove to yourself that ammonium nitrate also contains 5.037% H and 59.97% O by mass! (These percentages should sum to approximately 100%, but there may be roundoff error. In this example, the percentages sum to 100.007%)

Try this second example on your own. It's simpler than the NH_4NO_3 example. *Calculate the percentage composition by mass of table salt, NaCl.*

Answer: The percentage composition is 39.3% by mass Na and 60.7% by mass Cl.

<u>Applications of chemical formulas: Formulas (Empirical) from mass data:</u>

What if we turn the situation around? Would it be desirable to know the **chemical formula** of a compound if we already knew something about its chemical makeup?

How can we find the chemical makeup? There are various techniques (most beyond the scope of this course) that can provide us with the percentage composition of an unknown substance. We will perform a laboratory experiment that will give us the percentage composition data for an oxide of magnesium, so you will become familiar with how **some** of this data can be collected.

In the real world, we often don't know what compound has been spilled at a site. One way we can find out is to analyze what's there and try to figure out if the compound is troublesome or not.

Let's take an example. You're a forensic scientist. *Barrels of a white, crystalline compound are found inside a suspected terrorist's residence. The compound is analyzed and found to contain* ***35.0% N***, ***5.0% H***, *and* ***60.0% O***. *What is the likely identity of the compound?*

Given: 35.0% N, 5.0% H, 60.0% O **Find: Identity (formula)**

This problem is very similar to the case where we needed to find a mass percentage from a chemical formula. In that problem, we started with a mole ratio (the chemical formula) and found a mass ratio (the percent composition). In **this** problem, we're starting with the mass ration and are trying to find the mole ratio..

First, assume **exactly** 100g of the substance. Like the last problem, it makes no mathematical difference what amount of substance you assume, but assuming 100g makes the math simpler. Calculate the mass of each element in 100 grams of the substance using the given percentages.

Nitrogen:	(35.0%)(**100g**) =	**35.0g N**
Hydrogen:	(5.0%)(**100g**) =	**5.0g H**
Oxygen:	(60.0%)(**100g**) =	**60.0g O**

To find the formula, we must take the **mass ratio** here (35.0:5.0:60.0) and convert it to a **mole ratio**. To do this, we convert each mass to moles using the atomic weight of each element..

$$35.0\text{g N}\times\frac{1\text{ mol N}}{14.00678\text{ g N}}=2.50\text{ mol N}$$

$$5.0\text{ g H}\times\frac{1\text{ mol H}}{1.00794\text{ g H}}=5.0\text{ mol H}$$

$$60.0\text{ g O}\times\frac{1\text{ mol O}}{15.9994\text{ g O}}=3.75\text{ mol O}$$

The chemical formula is $N_{2.5}H_{5.0}O_{3.75}$, but we write chemical formulas in ratios of small whole numbers. After all, this is a normal chemical formula and atoms are not divided into halves and quarters. We need to simplify the ratio so that it contains only whole numbers.

The easiest way to simplify a ratio like the one above is to **divide each number by the smallest number** (this guarantees that one of the numbers will be 1)!

Nitrogen:	2.50 mol N / 2.50 =	**1 mol N**
Hydrogen:	5.0 mol H / 2.50 =	**2 mol H**
Oxygen:	3.75 mol O / 2.50 =	**1.5 mol O**

This is better than what we had originally, but we still need to get rid of the 1.5. We can multiply the ratio again by a number that will eliminate the 0.5 (which is just ½) ... 2.

Nitrogen:	2(1 mol N) =	**2 mol N**
Hydrogen:	2(2 mol H) =	**4 mol H**
Oxygen:	2(1.5 mol O) =	**3 mol O**

The formula of the compound is $N_2H_4O_3$.

The chemical formula of ammonium nitrate (NH_4NO_3 - a white, crystalline substance used in the Oklahoma City bombing years ago) can be written as $N_2H_4O_3$. The presence of barrels of this compound in a suspected terrorist's residence is certainly suspicious, and further tests on the compound should be conducted to determine if the compound really is NH_4NO_3.

This technique has **limitations**. From mass data, the only thing we can find out about the chemical formula is the **empirical formula**. We had to make an educated guess in the example above to conclude that the compound was ammonium nitrate. We should confirm all such guesses with further experimental evidence like tests for chemical or physical properties.

What if we'd analyzed a compound and found out it had an empirical formula of CH_2? There's no real **molecule** with that formula. There **are** chemical compounds with the formulas C_2H_4 and C_3H_6. You'd need **more information** to decide what compound you really had - information like chemical or physical properties.

Summary

In this note pack, we have discussed how to relate a chemical formula to the composition of a compound by mass, and how to determine the empirical formula of a compound from mass composition data. You should realize that you can't determine the molecular formula of a compound from mass data without other information. However, the empirical formula is still very useful for identification purposes.