# Chapter 5 CHEMICAL UNITS AND MASS



We now return to the matter of mass. Or, actually, the mass of matter.

We last left mass in the minuscule world of the atom in Chapter 2 when we first introduced atomic mass. Now we are going to discuss masses of polyatomic things, including elemental forms and compounds. We begin with the atomic mass unit, u, but later we will come into the practical world of the gram. Mass is one of the most important measurements in chemistry and the mass of a sample allows us to calculate the number of molecules in the sample. Why do we want to? When we do chemical reactions, a specific number of molecules (or whatever chemical units) reacts with a specific number of other molecules. We need to know how many things are in a sample, but we cannot count individual chemical units because they are too small and too many. We also cannot directly measure u's since that unit is too small by itself. So, somewhere along the road, we've got to come up to grams (or some other unit) which we can measure easily. We've got to have a connection between grams of sample and how many chemical units are in the sample. The overall result is an important one: we cannot directly count how many molecules are in a sample, but we can measure how many. And, as we discussed in Chapter 1, we can only measure to some limit of certainty; that means we will be doing sigfigs for numbers of molecules and such.

## 5.1 Still stuck on u.

In Chapter 2, we discussed atomic mass units with respect to a single atom and also to an "average" atom. The average atom took into account the different isotopes and this gave us the atomic mass in u or the atomic weight without the u. Now we do polyatomics. For these, we use "molecular mass" or "formula mass", for which the units are again u. The terms "molecular weight" and "formula weight" will again be a relative value, the same number but without the unit u.

The molecular mass is the average mass of a single molecule in u's. This is easy to do: it's just the sum of the masses of the atoms in the molecule. Let's do an example: find the molecular mass of selenium difluoride, $SeF_2$. All that you need to do is add up the atomic masses of one Se and two F's, as shown below at left. Another example: find the molecular mass of sulfur trioxide, $SO_3$. This is obtained from the sum of the atomic masses of one S and three O's, as shown at right.

| | | | | | |
|---|---|---|---|---|---|
| $SeF_2$ | Se | 78.96 u | $SO_3$ | S | 32.07 u |
| | F | 19.00 u | | O | 16.00 u |
| | F | 19.00 u | | O | 16.00 u |
| | | 116.96 u | | O | 16.00 u |
| | | | | | 80.07 u |

This means that the average mass of one molecule of $SeF_2$ is 116.96 u and the average mass of one molecule of $SO_3$ is 80.07 u. (I keep saying average because we are using atomic masses, most of which are averages. This is a minor detail, and I won't continue saying average.)

For network compounds, there are no simple molecules and so the term formula mass applies. A formula mass is the sum of the atomic masses of the formula unit. For example, the formula mass of potassium chloride, KCl, is derived from the mass of one K and one Cl. The formula mass of silicon dioxide, $SiO_2$, is derived from the mass of one Si and two O's.

| | | | | | |
|---|---|---|---|---|---|
| KCl | K | 39.10 u | $SiO_2$ | Si | 28.09 u |
| | Cl | 35.45 u | | O | 16.00 u |
| | | 74.55 u | | O | 16.00 u |
| | | | | | 60.09 u |

Since KCl is ionic, some of you might think that we should be using the mass of one $K^+$ ion and the mass of one $Cl^-$ ion. That's a good point. The masses of these separate ions differ from their atomic masses by the mass of one electron (which is not much anyway). It turns out that this difference drops out for the ionic compound as a whole.

| | | |
|---|---|---|
| KCl | $K^+$ | 39.10 u minus one $e^-$ mass |
| | $Cl^-$ | 35.45 u plus one $e^-$ mass |
| | | 74.55 u, same as above |

This will ALWAYS be true for formula masses of ionic compounds: you just take the atomic masses off the Periodic Table and don't worry about who's got how many electrons.

Now that I've just told you that a network compound goes by "formula mass", I will now tell you that we don't normally make the distinction in routine use. We use the term "molecular mass" generically. Thus, many chemists might also say the molecular mass of KCl is 74.55 u even though it's a network ionic compound. If your instructor requires the distinction, then follow it.

TECHNICALITY. There's a technical point I need to make about sigfigs. Different instructors handle molecular masses a bit differently for sigfig purposes. Notice that I set up each of these examples as a simple addition. I used the sigfig rule for addition/subtraction which goes by the decimal place but, in real life, when you plug these into your calculator, you'll often be using the multiplication key. For example, the molecular mass of $SO_3$ could be entered on the calculator as $3 \times 16.00 + 32.07$. So is this really addition or is this really multiplication for sigfig purposes? I'll be treating it as an addition problem, but you need to know what your instructor calls it. Does it matter? It can: sometimes it affects the round-off decision. I can illustrate this with a very simple example, $P_4$. This is an allotrope of phosphorus which I mentioned in Chapter 2. What's the molecular mass for $P_4$?

Addition round-off method

| | | |
|---|---|---|
| $P_4$ | P | 30.97 u |
| | P | 30.97 u |
| | P | 30.97 u |
| | P | 30.97 u |
| | | 123.88 u |

(Rounded to second decimal according to +/- rule)

Multiplication round-off method

$P_4$ $4 \times 30.97\text{ u} = 123.9\text{ u}$

(Rounded to four sigfigs according to ×/÷ rule. The 4 is exact, so you go by 30.97, which has four sigfigs.)

The two values reflect a different limit of certainty. Since I'm doing addition method, I would give the mass as 123.88 u, but another instructor could be doing multiplication and use the value 123.9 u. Which is correct? Within the sigfig system, both can be considered correct but remember that the sigfig system is itself a compromise system. It is not unusual for two ways to give the same answer but with different numbers of sigfigs. Your job is to be clear on how your instructor wants you to handle these. Does it even matter? Sometimes. Not always. But, yes, sometimes.

OK, this ends the technicality.

Let me make a point about formulas with parentheses. I'll illustrate with calcium dihydrogen phosphate, $Ca(H_2PO_4)_2$. If you're into gardening, you may have used this stuff. It's one of the compounds in "superphosphate" fertilizer which is sold in stores. The formula unit consists of one calcium ion and two dihydrogen phosphate ions. The subscript two outside the parentheses means two times everything inside. For the mass of the formula unit, we add the masses of one Ca (40.08 u), four H's (1.008 u each), two P's (30.97 u each) and eight O's (16.00 u each). The formula mass is the sum, 234.05 u.

### 5.2 We jump to the real world.

In our real world we can see an object and we can measure its mass in grams or whatever. An atom is incredibly tiny, however, and any real sample has a zillion atoms. Actually, several zillions. I described this in Chapter 2 but this is a really big point so I'm repeating it. Atoms are incomprehensibly small. A real sample contains an incomprehensibly huge number of them. This is what Nature has given us: immensely huge numbers of infinitesimally tiny objects.

In science many years ago, they established a numerical unit for working with these massively huge numbers. A "numerical unit" is just a unit which means a number. The most common example of a numerical unit in common usage is a dozen. A dozen is 12. That's 12 of anything. Eggs, roses, donuts, etc. (Years ago, a dozen donuts was 13.) Another numerical unit is gross. A gross is 144. Of anything. Dozen and gross are numerical units.

Chemists also have a numerical unit for dealing with atoms and molecules, but the number itself is incredibly huge. Big. REALLY BIG. The unit is called a "mole". I admit that I've often thought this word sounds totally unimpressive for a number of humongous proportion, but that's the name they gave it and we're stuck with it. The mole is abbreviated mol. (The abbreviation knocks off one whole letter. Some abbreviation.) The numerical value of the mole is $6.02214129 \times 10^{23}$. Why such a strange number? Well, it's not straightforward. They set the system up based on a measured number of atoms in exactly 12 grams of $^{12}C$. There are reasons for that and we don't need to go there. The net result is that it's not a simple, whole number. It's also not an exact number because it's a measured value. So it's not like a dozen, which is defined to be exactly twelve. For a mole, there are sigfigs to consider. In typical work, it is rounded to $6.022 \times 10^{23}$, four sigfigs. That's the way we'll use it most of the time.

$$\text{mol} = 6.022 \times 10^{23}$$

As we saw at the end of Chapter 1, such a relationship can be written as two conversion factors.

$$\frac{\text{mol}}{6.022 \times 10^{23}} \quad \text{OR} \quad \frac{6.022 \times 10^{23}}{\text{mol}}$$

By the way, the numerical value $6.022 \times 10^{23}$ is called "Avogadro's number" after Avogadro who had nothing to do with the number itself.

$6.022 \times 10^{23}$ is huge. It's immense. It's very difficult to comprehend the size of that number. $6.022 \times 10^{23}$ of anything you can see is unthinkable. Consider one mole of the smallest thing you can see. How about a human hair, only a fraction of an inch long? That's not a lot, but a mole of those would weigh about a trillion tons, even without the dandruff. Now, apply this immensely huge number to an infinitesimally tiny molecule and you get something reasonable: one mole of water molecules occupies 1.2 tablespoons. I said it upstairs and I'll say it again:

> THIS IS WHAT NATURE HAS GIVEN US: IMMENSELY HUGE NUMBERS OF INFINITESIMALLY TINY OBJECTS.

You must catch the significance here! The mole is the numerical unit which connects a huge number of infinitesimally tiny molecules to our real world and realistic sample sizes. The mole is our basic, routine unit for "how many". This is what we commonly use day to day.

There is another consequence of this mole unit which allows us to connect atomic mass units to grams. A mole of u's is a gram.

$$\text{g} = 6.022 \times 10^{23}\ \text{u}$$

This likewise can be presented in two ways.

$$\frac{\text{g}}{6.022 \times 10^{23}\ \text{u}} \quad \text{OR} \quad \frac{6.022 \times 10^{23}\ \text{u}}{\text{g}}$$

The mole is our important, numerical link to how many atoms and to their mass in grams.

This brings us to "molar mass". Molar mass is the mass in grams of one mole of anything: it could be a mole of atoms or a mole of molecules or a mole of formula units. This will change the way we deal with mass. Until now, everything we did with mass was in u for one unit: the atomic mass of one atom or the molecular mass of one molecule or the formula mass of one formula unit. All of those were u's for one individual unit. Now, molar mass is the SAME NUMBER but in grams for one mole of those units. Compare this to our previous examples.

| | | |
|---|---|---|
| $SeF_2$ | 116.96 u for one molecule | 116.96 g for one mole of molecules |
| $SO_3$ | 80.07 u for one molecule | 80.07 g for one mole of molecules |
| KCl | 74.55 u for one formula unit | 74.55 g for one mole of formula units |
| $SiO_2$ | 60.09 u for one formula unit | 60.09 g for one mole of formula units |
| $P_4$ | 123.88 u for one molecule | 123.88 g for one mole of molecules |
| $Ca(H_2PO_4)_2$ | 234.05 u for one formula unit | 234.05 g for one mole of formula units |

A key point from all of the above examples is that the number of u for one molecule (or one formula unit) is the SAME NUMBER as the number of grams for one mole of those molecules (or one mole of those formula units). Why does the SAME NUMBER apply to both values? Because everything else drops out. I'll show you using selenium difluoride. Here's the full dimensional analysis string for calculating the molar mass of $SeF_2$ from its molecular mass.

$$\overbrace{\frac{116.96\ \text{u}}{\text{molecule of SeF}_2}}^{\text{molecular mass}} \times \frac{\text{g}}{6.022 \times 10^{23}\ \text{u}} \times \frac{6.022 \times 10^{23}\ \text{molecules of SeF}_2}{\text{mol of SeF}_2} = \overbrace{\frac{116.96\ \text{g}}{\text{mol of SeF}_2}}^{\text{molar mass}}$$

Notice that "molecule(s) of $SeF_2$", "u" and even "$6.022 \times 10^{23}$" all cancel and drop out. (Go ahead and cross them out.) The net result is that for any formula unit, the number of u for one unit is the SAME NUMBER as the number of grams for one mole of those units.

Although the numbers are the same, you need to keep in mind the distinction between the terms. Atomic mass, molecular mass and formula mass are for one unit. Molar mass is for one mole of those units. Remember this. A few more examples for emphasis, please.

| | | |
|---|---|---|
| Ne | 20.18 u for one atom | 20.18 g for one mole of atoms |
| $CO_2$ | 44.01 u for one molecule | 44.01 g for one mole of molecules |
| $(NH_4)_2SO_4$ | 132.15 u for one formula unit | 132.15 g for one mole of formula units |

In all cases, these mass relationships can be represented by either of two fractional forms for use as conversion factors. I won't show this for all examples above, but I'll just do the selenium difluoride example.

One molecule of $SeF_2$: 116.96 u

Conversion factors: $\dfrac{116.96\ \text{u}}{\text{molecule}}$ OR $\dfrac{\text{molecule}}{116.96\ \text{u}}$

One mole of $SeF_2$: 116.96 g

Conversion factors: $\dfrac{116.96\ \text{g}}{\text{mol}}$ OR $\dfrac{\text{mol}}{116.96\ \text{g}}$

The g/mol and mol/g conversions are used extensively, as you will see.

Let's move on to sample sizes other than one mole. Consider this problem: how many moles of tin atoms are in a sample of 17.49 g Sn?

From the Periodic Table, the molar mass for tin is 118.7 g, so our sample of tin has some fraction of a mole of atoms. We need to find out just how much. We can execute this problem by dimensional analysis (although you can also use some other way if you want).

The molar mass for tin means that mol Sn = 118.7 g Sn

which can be taken as $\dfrac{118.7\ \text{g}}{\text{mol}}$ OR $\dfrac{\text{mol}}{118.7\ \text{g}}$

Our calculation is a one-step problem starting from g and going to mol. We need the conversion factor on the right with mol upstairs and g downstairs in order to cancel g Sn.

path: g Sn $\rightarrow$ mol Sn

$$17.49\ \text{g Sn} \times \frac{\text{mol Sn}}{118.7\ \text{g Sn}} = 0.1473\ \text{mol Sn}$$

From this we see that our sample of 17.49 g Sn corresponds to 0.1473 mol Sn.

Remember that a mol is just a number. It's always a mol <u>of something</u>. Just like a dozen is always a dozen of something. In general, for calculations such as this, we deal with a <u>mole of formula units, whatever the formula unit may be</u>. This may not always be clear, so let me give some pointers on how to interpret a "mole of formula units". It depends on whether you have a molecular compound or a network compound. I'll illustrate these with some examples that we've worked with.

- If I write "mol Sn", it means a mole of Sn formula units. Tin is a metal and it exists as a metallic network; the formula unit is one atom of tin in the network. Thus, "mol Sn" means a mole of tin atoms in the network.
- If I write "mol $SeF_2$", it means a mole of $SeF_2$ formula units. This is a molecular compound, so the formula unit is one molecule. Thus, "mol $SeF_2$" means a mole of those molecules.
- If I write "mol KCl", it means a mole of KCl formula units. KCl is an ionic compound, so this is an ionic network. The formula unit is one $K^+$ cation and one $Cl^-$ anion. Thus, "mol KCl" means a mole of $\{K^+ + Cl^-\}$ formula units.
- If I write "mol $SiO_2$", it means a mole of $SiO_2$ formula units. $SiO_2$ is a covalent network compound and the chemical unit is the network. Thus, "mol $SiO_2$" means a mole of {Si + 2 O} formula units.

Keep these pointers in mind.

Although mol is our common unit for "how many", you can still do individual units by bringing in Avogadro. As an illustration, let's keep the tin example from above but we'll change the question: how many Sn atoms are in 17.49 g Sn?

To do this, we must execute one more step beyond mole. We must take mole to individual atoms by way of Avogadro.

path: g Sn → mol Sn → atoms Sn

$$17.49 \text{ g Sn} \times \frac{\text{mol Sn}}{118.7 \text{ g Sn}} \times \frac{6.022 \times 10^{23} \text{ atoms Sn}}{\text{mol Sn}} = 8.873 \times 10^{22} \text{ atoms Sn}$$

Notice that the answer is a huge number: there's an extremely large number of atoms in just a modest sample size.

The grams/moles conversion is one of the most common conversions you'll do. You'll need to be able to do it both ways, g → mol and mol → g. You need to use molar mass as the conversion factor. Here are two Examples, one in each direction, using carbon dioxide, $CO_2$.

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**Example 1.** How many moles are in 3.08 g $CO_2$? The molar mass is 44.01 g.

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The molar mass means mol $CO_2$ = 44.01 g $CO_2$

for which you can write the following.

$$\frac{44.01 \text{ g}}{\text{mol}} \quad \text{OR} \quad \frac{\text{mol}}{44.01 \text{ g}}$$

Set this up as for the Sn example earlier.

path: g $CO_2$ → mol $CO_2$

$$3.08 \text{ g } CO_2 \times \frac{\text{mol } CO_2}{44.01 \text{ g } CO_2} = 0.0700 \text{ mol } CO_2$$

. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

**Example 2.** What's the mass of 1.621 mol $CO_2$?

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The same conversion factors apply but now you need the one with mol in the denominator.

path: mol $CO_2$ → g $CO_2$

$$1.621 \text{ mol } CO_2 \times \frac{44.01 \text{ g } CO_2}{\text{mol } CO_2} = 71.34 \text{ g } CO_2$$

I cannot tell you enough: the grams-to-moles and moles-to-grams conversions are immensely important. These are so important that it <u>must become automatic</u> for you to know how to do both ways. Get used to this.

### 5.3 Percent composition

There's another aspect of masses which I need to bring up. This aspect goes back quite a few years in chemistry but it also ties to some of the methods which chemists today use in order to identify compounds.

We start with the notion of "percent composition". Percent composition is the percent by mass of an element in a compound. This gives a relative distribution of the mass of a compound among its different elements. I'll illustrate using sulfur trioxide, $SO_3$; from earlier in this Chapter, we know that this compound has a molecular mass of 80.07 u and a molar mass of 80.07 g. For purposes of percent composition, we can base the calculation on one molecule and work with u or we can base the calculation on one mole and work with grams. It doesn't matter: the numbers will come out the same. Let's do one molecule for now and work with u.

Of the 80.07 u in one molecule, 32.07 u were from the sulfur atom. What percent is that?

Percent composition of sulfur:

$$\frac{\text{mass of S:}}{\text{total mass:}} \qquad \frac{32.07 \text{ u}}{80.07 \text{ u}} \times 100\% = 40.05\%$$

This tells us that 40.05% of the mass of one $SO_3$ molecule is derived from the sulfur atom in the molecule.

You can do this for each element in a compound. For the oxygens in $SO_3$, you count all three O's. Of the 80.07 u in one $SO_3$ molecule, 3 × 16.00 u were from the three oxygen atoms. What percent is that?

Percent composition of oxygen:

$$\frac{\text{mass of O's:}}{\text{total mass:}} \qquad \frac{3 \times 16.00\ \text{u}}{80.07\ \text{u}} \times 100\% = 59.95\%$$

This tells us that 59.95% of the mass of the molecule is derived from the oxygen atoms.

Notice that the u drops out of the calculation. If you work with grams, then g will also drop out. In the end, everything comes out the same, so it doesn't matter which way you go.

You can make all of this into an equation. For any one element Q in some formula, the percent composition of Q is determined by the following.

$$\text{percent composition} = \frac{(\text{number of atoms of Q in formula}) \times (\text{atomic mass of Q})}{\text{mass of formula unit}} \times 100\%$$

That's the u version. You can use g instead. Notice how this equation relates exactly to what we did for the sulfur trioxide example.

Here, you can do one.

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**Example 3.** Find the percent composition of phosphorus in calcium dihydrogen phosphate, $Ca(H_2PO_4)_2$.

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We did its formula mass earlier: 234.05 u. Plug in.

number of atoms of P × atomic mass of P

↓ ↓

$$\frac{\underline{\qquad\qquad} \times \underline{\qquad\qquad}}{\underline{\qquad\qquad}} \times 100\% = \underline{\qquad\qquad}$$

↑

mass of formula unit

The answer is 26.46%. If you didn't get that answer, then figure out what happened. Did you remember the two outside the parentheses? The percent compositions for the other elements in calcium dihydrogen phosphate are 17.12% Ca, 1.723% H and 54.69% O. Go ahead and check those numbers, too.

Ideally, the percent compositions for all elements in a compound should add to exactly 100%. We deal in the real world of measurements and uncertainty, however, and things aren't always ideal. Go back to the $SO_3$ example. Add the percent compositions together for the S and the O's. You get 100.00%. OK, fine. Now add the percent compositions together for the elements in calcium dihydrogen phosphate. What did you get? You don't get exactly 100.00%. These things can happen. They're not wrong. They're just not perfect.

Percent compositions are usually measured using certain kinds of instrumentation. These processes are called elemental analysis. There are several important uses of elemental analysis. For example, when chemists prepare a new compound, they are required to provide experimental proof to support their claim. There are different ways of doing this for different kinds of compounds, but elemental analysis has been one of the most common methods. Let's say you claim to make a new compound and you claim to know what its formula is. You conduct an elemental analysis and measure the percent composition of one or more elements. You compare these experimental results to the calculated percent compositions using the same approach we did above. If you have a good match, this helps to support your claim. If not, you goofed. I'll give you a real example. In my research group we prepared a new compound which we proposed to have the lengthy formula $Mo_2C_{40}H_{73}N_2O_6P_3S_6$. (Don't ask me to name it.) We believed this to be the correct formula based on different instrumental evidence. Elemental analysis was done for carbon, hydrogen and nitrogen. (You don't have to do all the elements in the compound.) From the formula, you can calculate what the percent compositions should be. The experimental results were 41.0% C, 6.6% H and 2.3% N. They're close, and that's considered a satisfactory match for such a complicated case.

### 5.4 An empirical approach

Another use of elemental analysis is to work backwards: start with percent composition and work towards the formula. This is useful when dealing with an unknown compound. Unfortunately, this has limitations since it cannot give you the true formula by itself, but it does provide valuable clues for ultimately identifying many compounds. Let's do an example.

We'll look at a cold case: refrigerants. These are the fluids which make refrigerators and air conditioners operate. There are many different types and sizes of refrigerators and air conditioners, and there are many different refrigerants used depending upon the application and design. Many of the refrigerants which are used in applications for the general public are compounds of carbon and fluorine with hydrogen and/or chlorine atoms also in the molecule. Many of these compounds had been used for refrigeration (and for various sorts of other things, too) for years until they started getting into the upper atmosphere and messing with the ozone layer. Well, not all of them. In the past, many were called Freons, but Freon is a trademark name; nowadays they're generically called refrigerant or just R. There's a bunch of these compounds and the industry uses a number to identify them. (These are not their real chemistry names.) Previously, R-12, whose chemical formula is $CF_2Cl_2$, was one of the most widely used in automobile air conditioners; that one was fairly hazardous to the ozone layer and it was banned years ago although it may yet be in some older cars. Nowadays, automobile air conditioners use R-134a which is $C_2H_2F_4$. Many home air conditioners use R-22 which is $CHF_2Cl$; it's being phased out also and newer refrigerants based on mixtures are coming into use. It turns out that the chlorine atoms in the molecules render these compounds especially damaging to the ozone layer, so the compounds with chlorine are the ones being phased out fastest. Some of these compounds are also greenhouse gases which adds to the environmental problems.

By the way, if you want to know how air conditioners work, you can find this in Section 35.4.

OK, let's get back to elemental analysis. Let's say you have an unknown refrigerant compound and you need to find out which one it is. You conduct an elemental analysis and find that the compound is composed of the elements carbon, fluorine and chlorine. The percent compositions are 14.1% C, 44.6% F and 41.5% Cl. What is the formula of the compound? Notice that the numbers don't add to exactly 100.0%. Again, measurements aren't always perfect, but they should be close.

Here's the general gist. Percent composition reflects the distribution of the masses of the atoms of the different elements in the compound. From these mass distributions, we can derive a relative ratio of the numbers of atoms of the different elements. This ratio is our target.

We start with the relative mass distributions as given by the percent compositions.

$$14.1\%\ \mathrm{C}\ :\ 44.6\%\ \mathrm{F}\ :\ 41.5\%\ \mathrm{Cl}$$

Now, pick a sample size. Any size would work, but most people would choose 1 g or 100 g when dealing with percents. I pick 100. g. So, in 100. g of this compound, there are zillions of molecules, each containing one or more atoms of C, F and Cl. By the measured percent compositions, my 100. g sample is composed of 14.1 g total C mass, 44.6 g total F mass and 41.5 g total Cl mass scattered among all the molecules. This gives a mass ratio for the elements.

$$14.1\ \mathrm{g\ C}\ :\ 44.6\ \mathrm{g\ F}\ :\ 41.5\ \mathrm{g\ Cl}$$

We want to know how many moles each of these corresponds to, so we bring in molar mass for each element.

$$\frac{14.1\ \mathrm{g\ C}}{12.01\ \mathrm{g\ C/mol\ C}}\ :\ \frac{44.6\ \mathrm{g\ F}}{19.00\ \mathrm{g\ F/mol\ F}}\ :\ \frac{41.5\ \mathrm{g\ Cl}}{35.45\ \mathrm{g\ Cl/mol\ Cl}}$$

Now divide each to get the mole ratio.

$$1.17\ \mathrm{mol\ C}\ :\ 2.35\ \mathrm{mol\ F}\ :\ 1.20\ \mathrm{mol\ Cl}$$

Remember that these are total mole amounts for the various atoms present in the sample of 100. g. For a formula, we need a whole number ratio of atoms. Frequently by this stage you can see such a whole number ratio; you may already see in this case that we have a 1:2:1 ratio, but the numbers don't always work out this well. When that happens, choose the one element with the fewest moles and find the ratio of each other element to that one. I'll illustrate this procedure. Here, C has the fewest moles, so we'll find the numbers of F and of Cl relative to C.

F's per C

$$\frac{F}{C} = \frac{2.35}{1.17} = 2.01$$

Since measurements aren't always exact, we take 2.01 as meaning the whole number two. So there are two F atoms per C atom in the molecule.

Cl's per C

$$\frac{Cl}{C} = \frac{1.20}{1.17} = 1.03$$

We take 1.03 as meaning the whole number one. So there is one Cl atom per C atom in the molecule. We now have our target ratio of atoms in the molecule.

1 C : 2 F : 1 Cl

Unfortunately, this is as far as we can go with percent composition. No, this is not yet the formula and we still don't know what the compound is. Why? Because many formulas could have this ratio: $CF_2Cl$, $C_2F_4Cl_2$, $C_3F_6Cl_3$, $C_4F_8Cl_4$, etc. They all have this ratio. This is the limitation which I mentioned above: percent composition will get you a ratio but it won't guarantee you a true formula. You need more information. Fortunately, we can usually obtain more information by other methods. I'll show you one such method, but I need to pause and make two points first.

Our 1:2:1 example here was fairly easy to see, but not all are that easy. Some compounds have screwy ratios. Let's say you calculate a ratio of 1.00:1.50 for two elements. Remember the ratio still has to end up as whole numbers, which means 2:3 in this case. Another example could be 1.00:1.67, which corresponds to 3:5. Of course, there are many other ratios. Some can be tricky. Be careful.

The second point to note involves a new term. Once you derive the smallest, whole-number ratio of the elements in the compound, it can be written in formula format. Our 1:2:1 ratio above could be written as $CF_2Cl$. This formula format is called an "empirical formula". Unfortunately it looks like a regular chemical formula and this leads to confusion. An empirical formula is the smallest, whole-number ratio of elements in a compound. An empirical formula <u>may or may not</u> be the true chemical formula. The possibilities I mentioned upstairs, $CF_2Cl$, $C_2F_4Cl_2$, $C_3F_6Cl_3$ and $C_4F_8Cl_4$, all have the same empirical formula, $CF_2Cl$. This is quite general, although the possibilities may not always be real compounds. For another example, $C_2H_4$, $C_3H_6$, $C_4H_8$, $C_5H_{10}$, etc., all have the same empirical formula ($CH_2$), and all of these are real but different compounds.

A key point to introduce here is that <u>a compound's true chemical formula is some whole-number multiplier of its empirical formula</u>. I can write this as follows.

$$\text{true chemical formula} = \text{multiplier} \times \text{empirical formula}$$

By the way, that multiplier can be one; this means that the empirical formula is indeed the same as the true chemical formula. For example, the chemical formula for water and the empirical formula for water are the same, $H_2O$.

OK, back to where we were. I said there are experimental ways of connecting the element ratio (empirical formula) to the true chemical formula. One of the easiest is molar mass, since molar masses for many things can be measured. The molar mass from the real chemical formula is related to the mass of the empirical formula by the <u>same multiplier</u> as above.

$$\text{molar mass} = \text{multiplier} \times \text{mass of empirical formula}$$

I'll illustrate with the $CH_2$ examples which I just mentioned.

| | empirical formula | possible molecular formulas | | | |
|---|---|---|---|---|---|
| | $CH_2$ | $C_2H_4$ | $C_3H_6$ | $C_4H_8$ | $C_5H_{10}$ |
| multiplier: | | 2 | 3 | 4 | 5 |
| molar masses: | 14.03 g | 28.05 g | 42.08 g | 56.10 g | 70.13 g |

The bottom line is this: the formula multiplier is the same as the molar mass multiplier. If you can measure the molar mass, then you can determine the multiplier.

Returning to our $CF_2Cl$ example, let's say we measured the molar mass to be 173 g. What is the true chemical formula? The mass of the empirical formula, $CF_2Cl$, is 85.46 g. The molar mass, 173 g, is then a multiple of this.

$$173 \text{ g} = \text{multiplier} \times 85.46 \text{ g}$$

The multiplier calculates to be 2.02, but it must be a whole number; we conclude this to be two. This means that the true chemical formula is two times the empirical formula. The final answer is $C_2F_4Cl_2$.

Remember: percent composition can get you an empirical formula, but that may or may not be the true chemical formula. Other information, such as molar mass, is required to connect the empirical formula to the true chemical formula.

Let's bring in another problem and work it out from scratch. Let's do a sugar. We talked about sugars in Chapter 3, and I mentioned that they can have different isomers which have the same chemical formula. We can't do isomers here, but we can solve for a chemical formula.

. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

**Example 4.** Elemental analysis of an unknown sugar gave percent compositions of 40.6% C and 6.56% H; the rest is O. The molar mass was measured to be 150. g. What is the true formula of this sugar?

. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

What to do? We first need to determine the empirical formula from the percent compositions. Then, we connect this empirical formula to the true formula using the given molar mass.

For the empirical formula part, we have 40.6% C and 6.56% H as given directly. The percent composition for O is not given directly, but we know that percent compositions add to 100.0%.

$$100.0\% = 40.6\% + 6.56\% + ?\% \text{ for O}$$

From this we find 52.8% for O. Now, proceed just like the refrigerant problem earlier. It goes pretty much the same. I'll leave blanks for you to fill in.

The percent compositions are relative mass distributions. Based on a sample size of 100. g, this gives a mass ratio for the elements.

$$40.6 \text{ g C} : 6.56 \text{ g H} : 52.8 \text{ g O}$$

We convert the mass ratio to mole ratio, bringing in the molar masses of the elements.

$$\frac{40.6 \text{ g C}}{12.01 \text{ g C/mol C}} : \frac{6.56 \text{ g H}}{1.008 \text{ g H/mol H}} : \frac{52.8 \text{ g O}}{16.00 \text{ g O/mol O}}$$

Solve for each: 3.38 mol C : ________ mol H : ________ mol O

By now, you may or may not see how these mole numbers relate to a whole number ratio. We'll work through the full process regardless. Of the three, which mole value is the minimum? (Clue: C is not the minimum.) Set up the atom ratios, putting the minimum in the denominator.

C's per ____'s

$$\frac{C}{\_\_} = \frac{3.38}{\_\_\_\_} = \_\_\_\_\_\_\_\_$$

If you're confused by what to fill in, look back at the refrigerant problem.

____'s per ____'s

$$\frac{\_\_}{\_\_} = \frac{\_\_\_\_}{\_\_\_\_} = \_\_\_\_\_\_\_\_$$

Now, what whole number ratios are represented by this outcome? ____ C : ____ H : ____ O

That provides your empirical formula. Write the empirical formula here. ____________________

That was the hard part; now you're almost done. Relate your empirical formula to the true formula by a multiplier. The multiplier comes from the formula mass relationships.

molar mass = multiplier × mass of empirical formula

150. g = multiplier × ____________ g

Fill in the blank for the mass of the empirical formula. Then re-arrange the equation and solve for the multiplier. Enter it at right. ________________

Now, multiply your multiplier times your empirical formula, and you get the true formula. Write your final answer here for the true formula. ____________________

You're done. Would you like to check your answer? Go look up ribose or xylose, which are two isomers with this formula.

**Problems**

1. True or false.
   a. Avogadro's number is an exact, numerical value.
   b. One gram equals one mol of atomic mass units.
   c. The empirical formula of butane is $C_2H_5$.
   d. The empirical formula of disulfur dichloride is SCl.
2. What is the molecular weight or formula weight for each of the following?
   a. $Bi(OH)_3$ b. $(NH_4)_2CO_3$ c. $As_2(CH_3)_4$
3. What is the molecular mass or formula mass for each of the following?
   a. copper(II) permanganate b. dichlorine hexaoxide
4. What is the molar mass for each of the following?
   a. $CH_4S$ b. $Pt(NO_3)_2$ c. $HTeOF_5$
5. What is the molar mass for each of the following?
   a. selenium tetrafluoride b. cobalt(II) perchlorate
6. Citric acid has the formula $C_6H_8O_7$. What is the mass (in g) of 0.05043 mol of citric acid?
7. Fruit sugar (fructose) has the formula $C_6H_{12}O_6$.
   a. How many moles are present in 8.006 g of fructose?
   b. How many carbon atoms are present in 8.006 g of fructose?
8. What is the percent composition of sulfur in each of the following?
   a. $CH_4SO_3$ b. tetraphosphorus trisulfide
9. A binary, covalent compound has the following percent compositions: 23.4% B and 76.6 % Cl.
   a. What is the empirical formula?
   b. If the molar mass is 185 g/mol, what is the molecular formula?
10. A covalent compound of H, Si and F is 4.105% H and 57.20% Si.
   a. What is the empirical formula?
   b. If the molar mass is 98.21 g/mol, what is the molecular formula?